Magnetic Space Groups

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Dedicated to

**Tikva Sa’eeda**
may her memory be blessed

to our kids, **Usa Shoshana** and **Steven Yitzchak**, who have always done us proud.

and to our granddaughter
**Talia Sa’eeda**
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Preface

This work discusses the structure, symbols, and properties of magnetic space groups. While the focus is on three-dimensional magnetic space groups, we have included analogous information on the structure, symbols, and properties of one- and two-dimensional magnetic space groups.

Unlike Gaul, this work is divided into two parts. The first is a discussion of the structure of magnetic groups, the Opechowski and Guccione symbols for magnetic space groups and the explicit listing of elements of one representative group from each of the 7, 80, and 1651 types of groups in, respectively, the superfamilies of one- two- and three-dimensional magnetic space groups. The second part of this work is an extension of the classic work on space groups published in the \textit{International Tables for Crystallography, Volume A: Space-Group Symmetry}, my work on non-magnetic subperiodic groups published in the \textit{International Tables for Crystallography, Volume E: Subperiodic Groups}, and my work on international-like tables for magnetic subperiodic groups. A reader familiar with any of these tables should readily recognize most content and format of the magnetic space group tables presented here.

This book was not computer generated. It was hand-calculated, checked, and typed. Consequently, in a massive work as this, the probability of errors and/or typos is then not zero. The author would appreciate being informed of any errors and/or typos found.

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1. Magnetic Space Groups: Symbols and Elements

1.1 Introduction

Magnetic groups are symmetry groups of arrangements of non-zero magnetic moments (spins). These groups were introduced by Landau and Lifschitz (1951, 1957) by reinterpreting the operation of "change in color" in two-color (black and white) crystallographic groups as "time inversion." Crystallographic two-color groups of rotations had been given by Heesch (1930) and Shubnikov (1951). The 1651 types of two-color three-dimensional space groups were derived by Belov et al (1955, 1957) and by Zamorzaev (1953, 1957) and called Shubnikov groups. Koptsik (1966) applied these groups to determine crystallographic and physical properties of magnetic structures.

The three-dimensional magnetic space groups were rederived and a new list of symbols for 1191 types of magnetic space groups was given by Opechowski & Guccione (1965) (see also Opechowski, 1986; Litvin, 2001, and Section 1.3). This number plus 230 space group types gives 1421 types of magnetic groups. The 230 types of groups which are the direct product of a space group and the time inversion group are not magnetic groups as the time inversion element in each such group precludes non-zero magnetic moments. To include these groups, Opechowski (1986) used the concept of reduced magnetic superfamily of a space group (see Section 1.2) to give a total of 1651 types of groups commonly referred to as magnetic space groups.

The Opechowski & Guccione list consists of a listing of a symbol for one representative magnetic space group from each type. To uniquely specify the meaning of these symbols required a specification of one representative space group chosen...
It was suggested in these two papers that the original Opechowski-Guccione set of symbols should be modified so one could correctly interpret them using ITC-A instead of ITC52. Adopting this ill-advised suggestion would have required in the future a new modification of the Opechowski-Guccione set of symbols whenever changes were made to the coordinate triplets of the general positions in ITC-A. Consequently, the meaning of the original Opechowski-Guccione list of symbols was specified by Litvin (2001).

ITC52 has been replace by Volume A of the *International Tables for Crystallography* (1983) (abbreviated here as *ITC-A*). One finds that, for some space groups, the set of coordinate triplets of the general positions explicitly printed in *ITC-A* differs from that explicitly printed in *ITC52*. As a consequence, if one attempts to interpret the Opechowski-Guccione symbols using *ITC-A*, one will, in many cases misinterpret the meaning of the symbol (Litvin, 1997, 1998).

Using the Opechowski-Guccione symbols, a list of symbols of the 1651 superfamilies of magnetic space group types is given in Table 1.1. In distinction from previous listings, where only a set of symbols were given, we specify explicitly the meaning of each symbol (Litvin, 2001). That is, we specify a representative magnetic group of that type. This consists of specifying the coordinate system used, and then relative to that coordinate system, the translational subgroup of the group. We then explicitly give a set of coset representatives of the coset decomposition of the group

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1 It was suggested in these two papers that the original Opechowski-Guccione set of symbols should be modified so one could correctly interpret them using ITC-A instead of ITC52. Adopting this ill-advised suggestion would have required in the future a new modification of the Opechowski-Guccione set of symbols whenever changes were made to the coordinate triplets of the general positions in ITC-A. Consequently, the meaning of the original Opechowski-Guccione list of symbols was specified by Litvin (2001).
with respect to its translational subgroup.

In Section 1.2, the concept of reduced magnetic superfamily of a space group is reviewed. This concept provides for a sub-classification of magnetic space groups. This is followed, in Section 1.3, by a detailed explanation of the contents of Table 1.1., of the magnetic space group type symbols and elements. In Section 1.4 we list the changes in the symbols listed in Opechowski & Guccione (1965) and Opechowski (1986), and those of Table 1.1. A comparison of the symbols introduced by Opechowski & Guccione (1965) and those of Belov et al (1957) is discussed in Section 1.5. A side by side comparison is given in Table 1.4.

For one- and two-dimensional black and white space groups, see respectively, Neronova & Belov (1961) and Weber (1929), Heesch (1929), Cochran (1952) and Belov & Tarkhova (1956). The symbols used here for the superfamilies of one- and two-dimensional magnetic space group types are given in Table 1.1 along with a specification of a representative group of each type. A comparison of the symbols for these groups with that of black and white group symbols given by Niggli (1964) and Belov & Tarkhova (1956) are given in Table 1.2.
1.2 Magnetic Superfamily

Let $F$ denote a space group type. The reduced magnetic superfamily of the space group of type $F$ (Opechowski, 1986) consists of:

1) A group of type $F$.

2) The group $F1'$, where $1'$ denotes time inversion group consisting of the identity 1 and time inversion 1'.

3) All non-equivalent groups $F(D) = D + (F - D)1'$ where $D$ is a subgroup of index two of $F$. Groups of this type will also be denoted by $M$.

The third set of groups is divided into two subdivisions:

3a) Groups $M_1$, where $D$ is an equi-translational subgroup of $F$.

3b) Groups $M_n$, where $D$ is an equi-class subgroup of $F$.

A survey of the crystallographic groups of the magnetic superfamily of crystallographic groups of type $F$ will consist of a listing of a set of coset representatives called the standard set of coset representatives, of the decomposition of the group with respect to its translational subgroup, of one group, called the representative group, from the groups of type $F$, one group $F1'$, and each non-equivalent group $F(D)$.

Reference to the group $F$, $F1'$, or $F(D)$ will refer to

---

2 A magnetic superfamily as defined by Zamorzaev (1957) does not include groups of type $F$.

3 Only the relative lengths and mutual orientations of the translation vectors and the standard set of coset representatives with respect to an implied coordinate system are given. The absolute lengths of translation vectors, the position in space of the origin of the coordinate system and the orientation in that space of the basis vectors of the coordinate system are not explicitly given.
the listed group and to the group type $F$, $F1'$, or $F(D)$ to that group's type.

1.3 Tables of Magnetic Space Group Symbols and Elements

The format of Table 1.1 is:

1) Serial number of the magnetic space group type.

2) Symbol of the magnetic space group type.

3) Symbol of the group type of the subgroup $D$ of index two of $F$ for magnetic space groups $F(D)$, and the position and orientation of the group $D$ in the coordinate system of the group $F(D)$ [which is the same as the coordinate system of $F$].

4) The standard set of coset representatives of the decomposition of the magnetic space group with respect to its translational subgroup.

1.3.1 Serial Number

A three part number $N_1.N_2.N_3$ is used. $N_1$ is a sequential number for the group type to which $F$ belongs. This is the same numbering as given in both ITC52 and ITC-A for the two and three-dimensional space group types. $N_2$ is a sequential numbering of the magnetic space group types of the superfamily of $F$. Group types $F$ always have the assigned number $N_1.1.N_3$, and group types $F1'$ the assigned number $N_1.2.N_3$. $N_3$ is a global sequential numbering of the 7, 80, and 1651 types of groups in, respectively, the superfamilies of one- two- and three-dimensional magnetic space groups.

1.3.2 Magnetic Space Group Symbol

In Figures 1.1 we give a list of symbols and diagrams for the magnetic group lattices.
The relative lengths and mutual orientations of the translation vectors of the translational subgroups of magnetic space groups are the same as for space groups \( F \). These lattice parameters are given in Table 1.2 according to the crystal system of \( F \). In Table 1.3.1 we give the symmetry directions of symmetry operations represented by characters in the Hermann-Mauguin symbol of a magnetic space group implied by the characters position in the symbol. In Table 1.3.2 we give the symbols used as subindices on the symmetry operations which represent these symmetry directions.

The symbol for a group \( F \) is that symbol for the group type \( F \) given by Opechowski and Guccione (1965). This group \( F \) is uniquely defined by its translational subgroup and the coset representatives of the coset decomposition of the group with respect to its translational subgroup. These coset representatives, see Section 1.3.4 below, are given in Table 1.1. The symbol for a group \( F1' \) is that of the group type \( F \) followed by \( 1' \).

The symbol for a group \( M_T = F(D) = D + (F - D)1' \) is based on the symbol for the group \( F \). As \( D \) is an equi-translational subgroup of \( F \), i.e. the translational subgroup \( T^M_T \) of the magnetic group \( M_T \) is \( T \), the translational subgroup of \( F \). The translational part of the group symbol of a \( M_T \) group is then the same as that of the corresponding group \( F \).

A number or letter in the rotational part of the symbol of \( F \) appears unchanged in the symbol for \( M_T \) if it is associated with a coset representative of the group \( F \), in the coset decomposition of \( F \) with respect to \( T \), which is also an element contained in the subgroup \( D \). If not in \( D \), i.e. in \( F - D \), the number or letter appears in the symbol for \( M_T \) with a prime to denote that the element in \( M_T \) is coupled with \( 1' \). For example, the
orthorhombic space group \( F = \text{Pca2}_1 \) is listed as the three-dimensional magnetic space group number 29.1.198. This group is defined by an orthorhombic translational subgroup \( T = \text{P} \), see Figures 1.1-3D, and the standard set of coset representatives\(^4\)

\[
(1|000) \quad (m_x|\frac{1}{2},0,\frac{1}{2}) \quad (m_y|\frac{1}{2},0,0) \quad (2z|0,0,\frac{1}{2}),
\]

the coset decomposition of \( F \) with respect to \( T \) can then be written as:

\[
F = T + (m_x|\frac{1}{2},0,\frac{1}{2})T + (m_y|\frac{1}{2},0,0)T + (2z|0,0,\frac{1}{2})T.
\]

The magnetic space group 29.5.202 is a group \( M_1 \) whose symbol is \( \text{Pc'a'2}_1 \). In this case we have

\[
\text{Pc'a'2}_1 = \text{P2}_1 + (\text{Pca2}_1 - \text{P2}_1)'1'
\]

i.e. \( F = \text{Pca2}_1 \) and \( D = \text{P2}_1 \). The symbol " 2, " in the symbol for \( F = \text{Pca2}_1 \), refers to the coset representative \((2z|0,0,\frac{1}{2})\), and element in \( D = \text{P2}_1 \). Consequently the symbol appears unprimed in the symbol for \( M_1 (\text{Pc'a'2}_1) \) and the coset representative \((2z|0,0,\frac{1}{2})\) appears as an unprimed coset representative in the standard set of coset representatives of \( M_1 \). The symbols " c " and " a " in \( F = \text{Pca2}_1 \), refer to the coset representatives \((m_x|\frac{1}{2},0,\frac{1}{2})\) and \((m_y|\frac{1}{2},0,0)\), respectively, neither of which are contained in \( D \). Consequently both symbols appear primed in the symbol for \( M_1 (\text{Pc'a'2}_1) \) and the coset representatives \((m_x|\frac{1}{2},0,\frac{1}{2})\) and \((m_y|\frac{1}{2},0,0)\) appear as primed coset representatives in the standard set of coset representatives of \( M_1 \). The magnetic group \( \text{Pc'a'2}_1 \), then has the orthorhombic translational subgroup \( T = \text{P} \) and the standard set of coset representatives

\(^4\)We use the Seitz notation \((R|\tau(R) + t)\) for elements of a space group \( F \). "R" is a rotation or rotation-inversion, "t" is a translation of the translational subgroup \( T \) of \( F \), and "\( \tau(R) \)" is a non-primitive translation associated with "R". The coset representatives are taken to be of the form \((R|\tau(R))\) which then defines the \( \tau(R) \) associated with the \( R \).
(1 000)  (m_x|½,0,½)’   (m_y|½,0,0)’   (2_z|0,0,½).

The symbol for a group \(M_R = F(D) = D + (F - D)1'\) is also based on the symbol for the group \(F\). (This is in contradistinction to the “BNS” symbols of \(M_R\) groups (Belov, Neronova, & Smirnova (1955, 1957)) where the symbol for a \(M_R\) group is based on the symbol for the group \(D\), see below Section 1.5) As this is an equi-class magnetic group, half the translations of \(F\) are now coupled with 1' in \(M_R\) and half the translations remain unprimed in \(M_R\). The unprimed translations constitute the translational subgroup \(T^D\) of \(D\). We can write the coset decomposition of the translational subgroup \(T\) of \(F\) with respect to the translational subgroup \(T^D\) of \(D\) as

\[
T = T^D + t_a T^D
\]

where \(t_a\) is a translation of \(F\) which appears primed (coupled with 1') in \(M_R\). The translational subgroup of \(M_R\) can then be written as

\[
T^M_R = T^D + t_a T^D
\]

Symbols for the translational groups \(T\), the translational subgroups \(T^D\) of \(T\) used in the symbol for \(M_R\) groups, and the choice of the translations \(t_a\) for magnetic space groups is given in Figures 1.1.

The symbol for a magnetic group \(M_R = F(D)\) is based on the symbol of the group \(F\), and is also a symbol for the subgroup \(D\) of unprimed elements. The translational part of the symbol of \(F\) is replaced by the symbol for the translational subgroup \(T^D\) of \(D\). If a coset representative \((R|\tau(R))\) of \(T\) in \(F\) appears as the coset representative \((R|\tau(R)+t_a)\) of \(T^D\) in \(D\), then the number or letter corresponding to \((R|\tau(R))\) in the symbol for \(F\) is primed. If \((R|\tau(R))\) appears unchanged as a coset representative of \(T^D\) in \(D\),
then the number or letter corresponding to \((R|\tau(R))\) in the symbol for \(F\) is unchanged. The resulting symbol is a symbol for \(D\) based on the symbol for \(F\) and is also a symbol for the magnetic space group \(M_R = F(D)\). The symbol specifies not only \(D\) but also \(F\): By deleting the subindex on the translational part of the symbol and the primes on the rotational part one obtains the symbol specifying \(F\). Having specified \(D\) and \(F\) one has specified the group \(M_R = F(D)\). For example: Consider again the three-dimensional space group 29.1.198, \(F = Pca2_1\) where

\[
F = T + \left( m_x \frac{1}{2}, 0, \frac{1}{2} \right) T + (m_y \frac{1}{2}, 0, 0) T + (2z \left| 0, 0, \frac{1}{2} \right) T.
\]

The symbol for the \(M_R = F(D)\) group 29.7.204 is \(P_{2b}c'a'2_1\) and is based on the symbol for \(F\). The translational subgroup \(T^0\) of \(D\) is given by the symbol \(P_{2b}\) where \(t_a = b = (0,1,0)\). The two primed symbols \(c'\) and \(a'\) in \(P_{2b}c'a'2_1\) denote that the two coset representatives \((m_x \frac{1}{2}, 0, \frac{1}{2})\) and \((m_y \frac{1}{2}, 0, 0)\) that appear in the set of standard coset representatives of \(T\) in \(F\) appear as the coset representatives \((m_x \frac{1}{2}, 1, \frac{1}{2})\) and \((m_y \frac{1}{2}, 1, 0)\) in the set of standard coset representatives of \(T^0\) in \(D\). As the symbol \(2_1\) in \(P_{2b}c'a'2_1\) is not primed, the coset representative \((2z \left| 0, 0, \frac{1}{2} \right)\) of \(T\) in \(F\) remains unchanged as a coset representative of \(T^0\) in \(D\). We have then the subgroup:

\[
D = T^0 + \left( m_x \frac{1}{2}, 1, \frac{1}{2} \right) T^0 + (m_y \frac{1}{2}, 1, 0) T^0 + (2z \left| 0, 0, \frac{1}{2} \right) T^0.
\]

We note that these same coset representatives of \(T^0\) in \(D\) are also the coset representatives of the standard set of coset representatives of \(T^M_R\) in \(M_R\):

\[
M_R = T^M_R + \left( m_x \frac{1}{2}, 1, \frac{1}{2} \right) T^M_R + (m_y \frac{1}{2}, 1, 0) T^M_R + (2z \left| 0, 0, \frac{1}{2} \right) T^M_R
\]

and consequently the standard set of coset representatives of \(P_{2b}c'a'2_1\) listed in the tables is:
(1|0,0,0)  (m_x|½,1,½)  (m_y|½,1,0)  (2_z|0,0,½)

Also, since $T^M_R = T^0 + t_a \cdot T^0$ it follows that:

$$M_R = D + (F-D)1'$$

$$M_R = (1|0,0,0) \cdot T^0 + (m_x|½,1,½) \cdot T^0 + (m_y|½,1,0) \cdot T^0 + (2_z|0,0,½) \cdot T^0 +$$
$$+ (1|0,1,0) \cdot T^0 + (m_x|½,0,½) \cdot T^0 + (m_y|½,0,0) \cdot T^0 + (2_z|0,1,½) \cdot T^0$$

Consequently, a primed number or letter in the symbol for $M_R$ (which is a symbol for $D$) denotes that the corresponding coset representative appears in $D$ coupled with $t_a$ and primed in $(F-D)1'$, e.g. $a'$ in $P_{2b} c'a'2_i$ denotes that the coset $(m_x|½,0,½)$ appears as $(m_x|½,1,½)$ in $D$ and as $(m_x|½,0,½)'$ in $(F-D)1'$. An unprimed number or letter in the symbol for $M_R$ (which is a symbol for $D$) denotes that the corresponding element appears unchanged in $D$ and coupled with $t_a$ and primed in $(F-D)1'$, e.g. the symbol $2_i$ in $P_{2b} c'a'2_i$ denotes that $(2_z|0,0,½)$ is in $D$ and $(2_z|1,0,½)'$ in $(F-D)1'$.

1.3.3 Symbol of the subgroup $D$

The third column contains the group type symbol of the subgroup $D$ of index two of the magnetic group $M = F(D)$.

a) For $M_T$ groups, the subgroup $D$ is defined by the translational subgroup $T$ of $F$ and the unprimed coset representatives listed in the fourth column.

b) For $M_R$ groups, $D$ is defined by the translational subgroup $T^0$ and the set of all coset representatives listed in the fourth column.

While the group type symbol of $D$ is given, the coset representatives of the subgroup $D$ of $M_T$ or $M_R$ defined in a) or b), respectively, may not be identical with the
standard set of coset representatives of the group $D$ found in the listing of the magnetic space groups. Consequently, to show the relationship between this group $D$ and the group of type $D$ listed in the tables, additional information is provided to define a new coordinate system in which the coset representatives of this subgroup of type $D$ are identical with the standard set of coset representatives listed for the group $D$.

Let $(O; a, b, c)$ be the coordinate system in which the three-dimensional space group $F$ is defined. “$O$” is the origin of the coordinate system, and $a$, $b$, and $c$ are the basis vectors of the coordinate system. $a$, $b$, and $c$ represent a set of basis vectors for a primitive cell for primitive lattices and for a conventional cell for centered lattices. A second coordinate system is defined by $(O+t; a', b', c')$. The origin is first translated from $O$ to $O+t$, and then the basis vectors $a$, $b$, and $c$ are changed to $a'$, $b'$ and $c'$ (for details, see Appendix 1.1).

Immediately following the group type symbol for the subgroup $D$ of $F$ we give a coordinate system $(O+t; a', b', c')$ [In the tables, for typographical simplicity, the symbols “$O+$” are omitted.] in which the coset representatives of the subgroup $D$ of $F$ are identical with the standard set of coset representatives of the group $D$ found in the listing of the magnetic space groups. $t$, $a'$, $b'$, and $c'$ are given in terms of the basis vectors of the coordinate system $(O; a, b, c)$ of the group $F$.

Example 1: For the $M_r$ magnetic group 10.4.52 = P2/m' one finds in the tables:

\[
P2 \quad (0,0,0; a, b, c) \quad (1|0,0,0) \quad (2\gamma|0,0,0) \quad (1|0,0,0)' \quad (m\gamma|0,0,0)'
\]
The translational subgroup of $\mathbf{D}$ is generated by the translations $(1|1,0,0)$, $(1|0,1,0)$, and $(1|0,0,1)$ of $\mathbf{T}$ since this is a $\mathbf{M}_r$ magnetic group, and the coset representatives of this group are $(1|0,0,0)$ and $(2_y|0,0,0)$, the unprimed coset representatives on the right. This subgroup $\mathbf{D}$ is of type P2. In the tables, listed for the group 3.1.8 $\mathbf{P}2$, one finds the identical two coset representatives. Consequently, there is no change the coordinate system, i.e. $t=(0,0,0)$ and $a'=a$, $b'=b$, and $c'=c$. In the coordinate system of the magnetic group P2/m', the coset representatives of its subgroup $\mathbf{D}$, of the type P2, are identical with the coset representatives of the group P2 found in the tables.

Example 2: For the $\mathbf{M}_r$ three-dimensional magnetic space group 16.7.105 $P_{2c}22'2'$ one finds in the tables:

$\mathbf{P22}_{11}$ $(0,0,0; a, b, 2c) \quad (1|0,0,0) \quad (2_x|0,0,0) \quad (2_y|0,0,1) \quad (2_z|0,0,1)$

The translational subgroup of $\mathbf{D}$ is generated by the translations $(1|1,0,0)$, $(1|0,1,0)$, and $(1|0,0,2)$, the generators of the unprimed subgroup of $\mathbf{T^M}_r$, and the coset representatives of this group are all those coset representatives on the right. This subgroup $\mathbf{D}$ is of type P221. In the tables, listed for the group 17.1.106 $\mathbf{P22}_{1}$ one finds a different set of coset representatives:

$(1|0,0,0) \quad (2_x|0,0,0) \quad (2_y|0,0,\frac{1}{2}) \quad (2_z|0,0,\frac{1}{2})$

Consequently, to show the relationship between the subgroup $\mathbf{D}$ of type P221 and the
listed group \( \text{P222}_1 \), we change the coordinate system in which \( D \) is defined to 
\((0,0,0; a, b, 2c)\). In this new coordinate system the coset representatives of \( D \) are identical with the coset representatives of the representative group \( \text{P222}_1 \).

Example 3: For the \( \text{M}_1 \) magnetic group \( 18.4.116 \ \text{P2}_2,2'\,2' \) one finds in the tables:

\[
\text{P2}_1 \ (0, \frac{1}{4}, 0 ; c, a, b) \quad (1 | 000) \quad (2_x | \frac{1}{2}, \frac{1}{2}, 0) \quad (2_y | \frac{1}{2}, \frac{1}{2}, 0)' \quad (2_z | 000)'
\]

The translational subgroup of \( D \) is generated by the translations \((1 | 0, 0, 1), (1 | 1, 0, 0), \) and \((1 | 0, 1, 0)\), and the coset representatives of this group are \((1 | 000)\) and \((2_x | \frac{1}{2}, \frac{1}{2}, 0)\), the unprimed coset representatives on the right. The group \( D \) is of type \( \text{P2}_1 \). In the tables, for the group \( 4.1.15 \ \text{P2}_1 \) one finds a different set of coset representatives, \((1 | 0, 0, 0)\) and \((2_y | 0, \frac{1}{2}, 0)\). Consequently, to show the relationship between the subgroup \( D \) of type \( \text{P2}_1 \) and the listed group \( \text{P2}_1 \), we change the coordinate system in which the subgroup \( D \) is defined to \((0, \frac{1}{4}, 0 ; c, a, b)\). The origin is first translated from \( O \) to \( O + t \), where \( t = (0, \frac{1}{4}, 0) \) and the a new set of basis vectors, \( a' = c, b' = a, \) and \( c' = b \) is defined. In this new coordinate system the coset representatives of the subgroup \( D \) are identical with the standard set of coset representatives of the representative group \( \text{P2}_1 \).

1.3.4 Coset Representatives

The groups listed are defined by their translational subgroups and a set of coset representatives, the standard set, of the coset decomposition of each group with
respect to its respective translational subgroup. The defining coset representatives are listed on the right hand side of Tables 1.1.

A two- or three-dimensional space group $F$ is defined by its translational subgroup and the set of coset representatives implied by the coordinates of the set of equivalent positions explicitly listed $ITC52$. For example, The three-dimensional space group $F = P222_1$ (17.1.106) has a primitive translational subgroup generated by $(1|0,0,0)$, $(1|0,1,0)$, and $(1|0,0,1)$. The coordinates of the set of equivalent positions listed in $ITC52$ under the group type $P222_1$ are:

$$x, y, z; \quad x, y, z; \quad x, y, z; \quad x, y, z; \quad x, y, z$$

The coset representative $(R | \tau(R))$ corresponding to a specific equivalent position $r' = x', y', z'$ is given by the equation $r' = (R | \tau(R))r = Rr + \tau(R)$. Corresponding to the preceding equivalent positions are the coset representatives

$$(1|0,0,0); \quad (2|x|0,0,0); \quad (2|y|0,0,1); \quad (2|z|0,0,1),$$

which are listed in Table 1.1.

The coset representatives of groups $F1'$ are not explicitly given. These are taken as the coset representatives of $F$ plus each of these coset representatives multiplied by 1'. For example, the coset representatives of $F = P222_1$ are given above. The coset representatives of $F1' = P222_1 1'$ are
(1|0,0,0); (2x|0,0,0); (2y|0,0,½); (2z|0,0,½),
(1|0,0,0)'; (2x|0,0,0)'; (2y|0,0,½)'; (2z|0,0,½ ).

The coset representatives of groups \( M_T = F(D) \) are derived from the coset representatives of \( F \). Each coset representative of \( F \) appears unchanged or primed, see Section 1.3.2 above, as a coset representative of \( M_T \). For example, The coset representatives of \( F = P222 \) are

(1|0,0,0); (2x|0,0,0); (2y|0,0,½); (2z|0,0,½).

The coset representatives of \( M_T = P2'2'2 \) are:

(1|0,0,0); (2x|0,0,0)'; (2y|0,0,½)'; (2z|0,0,½).

The coset representatives of groups \( M_R = F(D) \) are also derived from the coset representatives of \( F \). They are also chosen such that they are also coset representatives of \( D \) with respect to its subgroup \( T^0 \). Each coset representative of \( F \) appears either unchanged or multiplied by \( t_0 \), see Section 1.3.2 above. For example:
The coset representatives of \( F = P222 \) are

(1|0,0,0); (2x|0,0,0); (2y|0,0,½); (2z|0,0,½).

SECTION 1 - 15
The coset representatives of $M_R = P_{2a}2'2'2_1$, where $t_a = (1,0,0)$, are:

$$(1|0,0,0); \quad (2_x|1,0,0); \quad (2_y|1,0, \frac{1}{2}); \quad (2_z|0,0,\frac{1}{2}).$$

### 1.4 Changes in Symbols

Typographical errors in Opechowski & Guccione (1965) corrected in Opechowski (1986) of three-dimensional magnetic space group types are as follows:

<table>
<thead>
<tr>
<th>Numbering in Table 1.1</th>
<th>Opechowski &amp; Guccione (1965)</th>
<th>Opechowski (1986)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16.4.102</td>
<td>$P_{2a}222$</td>
<td>$P_{2a}222$</td>
</tr>
<tr>
<td>43.4.323</td>
<td>$F_{dd}d'2$</td>
<td>$F_{d'd}2$</td>
</tr>
<tr>
<td>47.6.352</td>
<td>$P_{2a}mmm$</td>
<td>$P_{2a}mmm$</td>
</tr>
<tr>
<td>67.17.593</td>
<td>$C_{1}m'm'a'$</td>
<td>$C_{1}m'm'a'$</td>
</tr>
<tr>
<td>108.8.899</td>
<td>$I_4'c'm'$</td>
<td>$I_p\ 4'c'm'$</td>
</tr>
<tr>
<td>108.9.900</td>
<td>$I_4c'm'$</td>
<td>$I_p\ 4c'm'$</td>
</tr>
<tr>
<td>124.1.1018</td>
<td>$P4/mcr$</td>
<td>$P4/mcc$</td>
</tr>
<tr>
<td>132.4.1113</td>
<td>$P_{4_2}/mcm'$</td>
<td>$P_{4_2}/'mcm'$</td>
</tr>
</tbody>
</table>

In both Opechowski & Guccione (1965) and Opechowski (1986) the symbol $P_{2b} c'ca$ is listed twice, in the numbering of Table 1.1, at entries 54.11.438 and 54.13.440. The second has been changed to $P_{2b} c'ca'$, a magnetic group which has a non-magnetic subgroup of the type $Pnna$.

Three more changes have been made:
Numbering in Table 1.1  Opechowski & Guccione (1965)  Table 1.1  Opechowski (1986)

131.13.1109  \( P_4 \frac{4}{m'mc} \)  \( P_p 4_2'/m'mc' \)

177.7.1385  \( P_{2c} 6'22 \)  \( P_{2c} 6'22' \)

180.7.1402  \( P_{2c} 6_2'22 \)  \( P_{2c} 6_2'22' \)

The reason for these changes are similar: For the middle case, the group \( P622 \) is listed in Table 1.1 as

\[
\begin{align*}
177.1.1379 & \quad P622 \\
\{ & 1 \mid 0,0,0 \} \quad \{ & 3 \mid 0,0,0 \} \quad \{ & 3^{-1} \mid 0,0,0 \} \\
\{ & 2 \mid 0,0,0 \} \quad \{ & 6 \mid 0,0,0 \} \quad \{ & 6^{-1} \mid 0,0,0 \} \\
\{ & 2 \mid 0,0,0 \} \quad \{ & 2_y \mid 0,0,0 \} \quad \{ & 2_y \mid 0,0,0 \} \\
\{ & 2 \mid 0,0,0 \} \quad \{ & 2 \mid 0,0,0 \} \quad \{ & 2 \mid 0,0,0 \}
\end{align*}
\]

177.7.1385 is a group with a \( P_{2c} \) lattice. The symbol 6' means that the coset representative \( (6_z \mid 0,0,0) \) in the standard set of coset representatives of the coset decomposition of \( P622 \) with respect to \( P \) (listed in 177.1.1379) appears as \( (6_z \mid 0,0,1) \) in the standard set of coset representatives of the coset decomposition of the magnetic group with respect to \( P_{2c} \). This implies the following coset representatives of 177.7.1385:

\[
\begin{align*}
\{ & 1 \mid 0,0,0 \} \quad \{ & 3 \mid 0,0,0 \} \quad \{ & 3^{-1} \mid 0,0,0 \} \\
\{ & 2_z \mid 0,0,1 \} \quad \{ & 6_z \mid 0,0,1 \} \quad \{ & 6_z^{-1} \mid 0,0,1 \}
\end{align*}
\]

The unprimed symbol 2 following the 6' implies that the coset representative \( (2_z \mid 0,0,0) \) remains the same as a coset representative in 177.7.1385. Combining this with the
listed coset representatives implies the complete set of coset representatives found in Table 1.1:

\[
\begin{align*}
(1 | 0,0,0) & \quad (3_{z} | 0,0,0) & \quad (3_{z}^{-1} | 0,0,0) \\
(2_{z} | 0,0,1) & \quad (6_{z} | 0,0,1) & \quad (6_{z}^{-1} | 0,0,1) \\
(2_{x} | 0,0,0) & \quad (2_{xy} | 0,0,0) & \quad (2_{y} | 0,0,0) \\
(2_{1} | 0,0,1) & \quad (2_{2} | 0,0,1) & \quad (2_{3} | 0,0,1)
\end{align*}
\]

Note that the coset representative \((2_{1} | 0,0,0)\) of the coset decomposition of \(P622\) with respect to \(P\) now appears as the coset representative \((2_{1} | 0,0,1)\) in the coset decomposition of the magnetic group 177.7.1385 with respect to \(P_{2c}\). Consequently, the second symbol 2 in \(P622\), appears as 2’ in the symbol of 177.7.1385, i.e. the symbol of this magnetic group is \(P_{2c}6_{2}’22’\).

1.5 Relationship to Black and White Space Group Symbols

Opechowski & Guccione symbols (1965) for all group types in a three-dimensional magnetic superfamily of type \(F\) are based on the symbol of the three-dimensional space group \(F\). For groups \(F\), \(F1’\), and \(M_{F}\), the Belov et al (1955, 1957) symbols do the same. However, for groups of the type \(M_{R} = F(D) = D + (F - D)1’\) Belov et al (1955, 1957) base their symbol on the symbol for the group \(D\), the unprimed subgroup of index 2. For example, the Opechowski & Guccione symbol for group 47.11.357 is \(P_{c}mmm’\). From this we have that \(F = Pmmm\) and from Table 1.1 that \(D = Cmma\). The Belov et al symbol for this group 47.11.357 is based on the symbol of the subgroup \(D\), i.e. the symbol Cmma: A group \(M_{R}\) can be written as \(M_{R} = F(D) = D + t_{a}’ D\), where \(t_{a}\) is a translation of \(F\) not in \(D\). For the group 47.11.357, this translation is chosen as \(a = (1,0,0)\) and is found in the figure for the \(P_{c}\) lattice in Figures 1.1. The
translational subgroup of this group is symbolically represented by Belov et al as $C_a$ where $C$ represents the translational subgroup of $D = C_{mma}$ and the subscript "a" denotes the translation $t_a = a$. This leads to the Belov et al symbol of $C_a m'm'a$ for the group 47.11.3 57.

A side by side comparison of Opechowski & Guccione symbols for three-dimensional magnetic space groups and Belov et al symbols for three-dimensional black and white space groups is given in Table 1.4-3D. As the Belov et al symbols for groups of type $F, F'$ and $M_r$ are the same as Opechowski & Guccione symbols, we list Belov et al symbols explicitly only for groups of type $M_r$. Comparisons of one- and two-dimensional magnetic space groups and black and white space groups are given, respectively, in Tables 1.4-1D and 1.4-2D.
2. Guide to the use of the magnetic space groups tables

2.1 Introduction

In this section we present a guide to the tabulation of properties of the superfamilies of one-, two-, and three-dimensional magnetic space groups given, respectively, in Table 3 - 1D, Table 3 - 2D, and Table 3 - 3D. The format and content of these magnetic group tables are similar to the format and content of the space group tables in *ITC-A: International Tables for Crystallography, Volume A* (1983), the subperiodic group tables in *ITC-E: International Tables for Crystallography, Volume E* (2002), and the same as that in the magnetic subperiodic group tables (Litvin, 2005).

2.2 Contents of the Magnetic Space Group Tables

The content of the magnetic group tables consists of the following:

(1) Lattice Diagram

(2) Headline

(3) Diagrams of symmetry elements and of the general positions

(4) Origin

(5) Asymmetric unit

(6) Symmetry operations

(7) Generators selected

(8) Positions, with multiplicities, site symmetries, coordinates, and magnetic moments

(9) Symmetry of special projections
2.2.1 Lattice Diagram

In the upper left hand corner of the first page of tables for each magnetic space group is the lattice diagram of the magnetic space group. This lattice diagram depicts the coordinate system used, the conventional unit cell of the space group $F$, the magnetic space group's magnetic superfamily type, and the generators of the translational subgroup of the magnetic space group. For example, in Figures 2.2.1.1 and 2.2.1.2 we show the lattice diagrams for the orthorhombic magnetic space groups $Pmc2_1$ and $P_{2b}m'c'2_1$, respectively. The generating lattice vectors depicted are color coded. Those colored black are not coupled with time inversion while those colored red are coupled with time inversion. In the former group $Pmc2_1$, a magnetic group of the type $F$, the lattice is an orthorhombic "P" lattice, see Figures 1.1, and no generating
translation is coupled with time in version. In the latter group $P_{2b} m'c'2_1$, a magnetic
group of type $M_R$, the lattice is an orthorhombic "$P_{2b}$" lattice, with the generating lattice
vector in the y-direction coupled with time inversion.

2.2.2 Headline

To the right of the lattice diagram is a two line heading, an example is given in
Figure 2.2.2.1. On the upper line, starting on the left, are three entries:

<table>
<thead>
<tr>
<th>P4/m'nm</th>
<th>4/m'nm</th>
<th>Tetragonal</th>
</tr>
</thead>
<tbody>
<tr>
<td>123.3.1001</td>
<td>P4/m'2'/m2'/m</td>
<td></td>
</tr>
</tbody>
</table>

Figure 2.2.2.1: Headline of magnetic space group P4/m'nm.

(1) The short international (Hermann-Mauguin) symbol of the magnetic space
group. Each symbol has two meanings: The first is that of the Hermann-Mauguin
symbol of a magnetic space group type. The second is that of a specific magnetic
space group which belongs to this magnetic space group type. Given a coordinate
system, this group is defined both by the list of symmetry operations (see Section 2.2.6)
given on the page with this Hermann-Mauguin symbol in the heading, or by the given
list of general positions and magnetic moments (see Section 2.2.8).

(2) The short international (Hermann-Mauguin) point group symbol for the
geometric class to which the magnetic space group belongs.

(3) The crystal system to which the magnetic space group belongs.

The second line has two additional entries:

(1) The three part numerical serial index of the magnetic space group (see
(2) The long international (Hermann-Mauguin) symbol of the magnetic space group.

2.2.3 Diagrams of symmetry elements and of the general positions

There are two types of diagrams, symmetry diagrams and general position diagrams. The symmetry diagrams show (1) the relative locations and orientations of the symmetry elements and (2) the locations and orientations of the symmetry elements relative to a given coordinate system. The general position diagrams show, in that coordinate system, the arrangement of a set of symmetrically equivalent points and relative orientations of magnetic moments on this set of equivalent points relative to the symmetry elements.

For the three-dimensional magnetic space groups, all diagrams are orthogonal projections and the projection direction is along the \( c \) basis vector, see Table 1.2. If the other two basis vectors are not parallel to the plane of the diagram, they are indicated by a subscript "p", e.g. \( a_p \) and \( b_p \). Schematic representations of the diagrams, showing their conventional coordinate system, i.e. the origin "O" and basis vectors, are given in Figures 2.2.3.1. The general position diagram is shown on the left and indicated by the letter "G". The symmetry diagram is on the right.

The graphical symbols used in the symmetry diagrams are listed in Table 2.2.3 and are an extension of those used in ITC-A (1983), ITC-E (2002) and Litvin (2005). For three-dimensional magnetic space groups, the symmetry planes and symmetry axes parallel to the plane of diagram, for rotoinversions, and for centers of symmetry, the "heights" \( h \) along the projection direction above the plane of the diagram are given.
The heights are given as fractions of the shortest translation along the projection direction and if different from zero, are printed next to the graphical symbol, see e.g. Figure 2.2.3.2.

**Figure 2.2.3.2:** Symmetry diagram of the three-dimensional magnetic space group $P4_{1}2'2'$

In the general position diagrams, the general positions and corresponding magnetic moments are color coded. Positions with a z-component of "+z" are circles color coded red and with a z-component of "-z" are circles color coded blue. If the z-component is either "h+z" or "h-z" with $h \neq 0$, then the height "h" is printed next to the general position, e.g. $\frac{1}{4}$. If two general positions have the same x-component and y-component, with z-components +z and -z, respectively, the positions are denoted as . The magnetic moments are color coded to the general position to which they are associated, their direction in the plane of projection is given by an
arrow in the direction of the magnetic moment. A "+" or "-" sign near the tip of the arrow indicates the magnetic moment is inclined, respectively, above or below the plane of projection, as in Figure 2.2.3.3.

![Figure 2.2.3.3: General position diagram of the three-dimensional magnetic space group P4,2'2'](image)

For magnetic space groups of the type F1', the symmetry diagram is that of the group F. That each symmetry element also appears coupled with time inversion is represented by a red 1' printed between and above the general position and symmetry diagrams. Because groups of this kind contain the time inversion symmetry, the magnetic moments are all identically zero, and no arrows appear in the general position diagram. An example, the diagrams of three-dimensional magnetic space group P4,221' are shown in Figure 2.2.3.4:
2.2.4 Origin

If the magnetic space group is centrosymmetric then the inversion center or a position of high site symmetry, as on the four-fold axis of tetragonal groups, is chosen as the origin. For noncentrosymmetric groups, the origin is at a point of highest site symmetry. If no symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetries.

In the Origin line below the diagrams, the site symmetry of the origin is given. An additional symbol indicates all symmetry elements that pass through the origin. For example, for the three-dimensional magnetic space group I4/mcm, one finds "Origin at center (4/m) at 4/mc2/c." The cite symmetry is 4/m and in addition, two glide planes perpendicular to the y- and z-axis, and a screw axis parallel to the z-axis pass through the origin.
2.2.5 Asymmetric Unit

An asymmetric unit of a magnetic space group is a simply connected smallest part of space from which, by application of all symmetry operations of the magnetic space group, exactly fills the whole space. Since the magnetic space groups contain a translational subgroup, the asymmetric unit is a finite part of space. We define the asymmetric unit by setting the limits on the coordinates of points contained in the asymmetric unit. For example, for the three-dimensional magnetic space group I4/m'cm (140.3.1198) one finds:

Asymmetric unit  \(0 < x < 1/2; \ 0 < y < 1/2; \ 0 < z < 1/4; \ y < 1/2 - x\)

Drawings showing the boundary planes occurring in the tetragonal, trigonal, and hexagonal systems, together with their algebraic equations are given in Figure 2.8.1 of ITC-A (1983). Drawings of asymmetric units for cubic groups have been published by Koch & Fisher (1974). The asymmetric units have complicated shapes in the trigonal, hexagonal, and cubic crystal systems and consequently are also specified by given the vertices of the asymmetric unit. For example, for the three-dimensional magnetic space group P6\(_3\)/m (176.1.1374) one finds:

| Asymmetric unit | \(0 \leq x \leq 2/3; \ 0 \leq y \leq 2/3; \ 0 \leq z \leq 1/4; \ x \leq (1+y)/2; \ y \leq \min(1-x,(1+x)/2)\) |
| Vertices | 0,0,0 | 1/2,0,0 | 2/3,1/3,0 | 1/3,2/3,0 | 0,1/2,0 |
| | 0,0,1/4 | 1/2,0,1/4 | 2/3,1/3,1/4 | 1/3,2/3,1/4 | 0,1/2,1/4 |
Because the asymmetric unit is invariant under time inversion, all magnetic space groups $\mathbf{F}$, $\mathbf{F}^*$, and $\mathbf{F}(\mathbf{D})$ of the magnetic superfamily of type $\mathbf{F}$ have identical asymmetric units.

2.2.6 Symmetry operations

Listed under the heading of Symmetry operations is the geometric description of the symmetry operations of the magnetic space group. In addition, each symmetry operation is also given in Seitz notation (Burns & Glazer, 1990). The corresponding coordinate triplets of the General positions may be interpreted as a second description of the symmetry operations, a description in matrix form. The numbering (1), (2), ..., (p), ... of the entries in the blocks Symmetry operations is the same as the numbering of the corresponding coordinate triplets of the General positions, the first block below Positions. For all magnetic space groups with primitive "P" lattices, the two lists, Symmetry operations and General positions, have the same number of entries.

For magnetic space groups with centered cells, only one block of several (2,3, or 4) blocks of the General positions is explicitly given. A set of (2,3, or 4) centering translations is given below the subheading Coordinates. Each of these translations is added to the given block of general positions to obtain the complete set of blocks of general positions. While one of the several blocks of general positions is explicitly given, the corresponding symmetry operations are all explicitly given. Each corresponding block of symmetry operations is listed under a subheading of "centering translation + set" for each centering translation listed below the subheading Coordinates.

A symbol denoting the geometric description of each symmetry operation is
given. Details of this symbolism, except for the use of prime to denote time inversion, are given in Section 11.2 of *ITC-A* (1983). For glide planes and screw axes the glide and screw part are always explicitly given in parentheses by fractional coordinates, i.e. by fractions of the basis vectors of the coordinate system of F of the superfamily of the magnetic group. A coordinate triplet indicating the location and orientation of the symmetry element is given, and for rotoinversions, the location of the inversion point is also given. These symbols, with the addition of a prime to denote time inversion, follow those used in *ITC-A* (1983), *ITC-E* (2002), and Litvin (2005).

2.2.7 Generators selected

The line *Generators selected* lists the symmetry operations selected to generate the symmetrically equivalent points of the General position from a point with coordinates x, y, z. The first generator is always the identity operation given by (1) followed by generating translations. Additional generators are given as numbers (p) which refer to the coordinate triplets of the General position and to corresponding symmetry operations in the first block, if more than one, of Symmetry operations.

2.2.8 Positions, with multiplicities, site symmetries, coordinates, and magnetic moments

The entries under Positions, referred to as Wyckoff positions, consists of the General positions, the upper block, followed by blocks of Special positions. The upper block of positions, the general positions, is a set of symmetrically equivalent points where each point is left invariant only by the identity operation or, for magnetic groups F1', by the identity operation and time inversion, but by no other
Symmetry operations of the magnetic space group. The lower blocks, the special positions, are a set of symmetrically equivalent points where each point is left invariant by at least one additional operation in addition to the identity operation, or , for magnetic space groups F1, in addition to the identity operation and time inversion.

For each block of positions information is provided:

**Multiplicity**: The multiplicity is the number of equivalent positions in the conventional unit cell of the non-magnetic group F associated with the magnetic space group.

**Wyckoff Letter**: This letter is a coding scheme for the blocks of positions, starting with "a" at the bottom block and continuing upwards in alphabetical order.

**Site symmetry**: The site symmetry group is the largest subgroup of the magnetic space group that leaves invariant the first position in each block of positions. This group is isomorphic to a subgroup of the point group of the magnetic space group. An "oriented" symbol is used to show how the symmetry elements at a site are related to the conventional crystallographic basis and the sequence of characters in the symbol correspond to the sequence of symmetry directions as in the magnetic space group symbol, see Table 1.3. Sets of equivalent symmetry directions that do not contribute any element to the site symmetry are represented by dots. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the 2c position of the three-dimensional magnetic space group P4'm'm (99.3.825) the site symmetry group is 2m'm'. where the two characters m'm' represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry directions.
Coordinates of Positions and Components of Magnetic Moments: In each block of positions, the coordinates of each position are given. Immediately following each set of position coordinates are the components of the symmetry allowed magnetic moment at that position. The components of the magnetic moment of the first position is determined from the given site symmetry group. The components of the magnetic moments at the remaining positions are determined by applying the symmetry operations to the components of that magnetic moment at the first position.

2.2.9 Symmetry of special projections

Under the heading Symmetry of special projections the following information is given for the projections of each magnetic space group:

**Projection direction:** All projections are orthogonal, i.e. the projection, for three-dimensional magnetic space groups, is onto a plane normal to the projection direction. The projection directions are:

- Triclinic, Monoclinic, Orthorhombic: [001] [100] [010]
- Tetragonal: [001] [100] [110]
- Hexagonal: [001] [100] [210]
- Rhombohedral: [111] [110] [211]
- Cubic: [001] [111] [110]

For two-dimensional magnetic space groups, the projection is onto a line normal to the projection direction. The projection directions are:
<table>
<thead>
<tr>
<th>Shape</th>
<th>Basis Vectors</th>
<th>Index 1</th>
<th>Index 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oblique</td>
<td>$\mathbf{a}^<em>\mathbf{, b}^</em>$</td>
<td>[10]</td>
<td>[01]</td>
</tr>
<tr>
<td>Rectangular</td>
<td>$\mathbf{a}^<em>\mathbf{, b}^</em>$</td>
<td>[10]</td>
<td>[01]</td>
</tr>
<tr>
<td>Square</td>
<td>$\mathbf{a}^<em>\mathbf{, b}^</em>$</td>
<td>[10]</td>
<td>[11]</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$\mathbf{a}^<em>\mathbf{, b}^</em>$</td>
<td>[10]</td>
<td>[21]</td>
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</tbody>
</table>

**Basis vectors**: For three-dimensional magnetic space groups, the relationship between the basis vectors $\mathbf{a}^*, \mathbf{b}^*$ of the two-dimensional magnetic space group symmetry of the projection is given in terms of the basis vectors $\mathbf{a, b, c}$ of the three-dimensional magnetic space group. For triclinic and monoclinic three-dimensional magnetic space groups where basis vectors $\mathbf{a, b, c}$ are inclined to the plane of projection, these basis vectors are replaced by $\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p$, respectively.

For two-dimensional magnetic space groups, the relationship between the basis vector $\mathbf{a}^*$ of the one-dimensional magnetic space group symmetry of the projection is given in terms of the basis vectors $\mathbf{a}$ and $\mathbf{b}$ of the two-dimensional magnetic space group. For oblique two-dimensional magnetic space groups where basis vectors $\mathbf{a}$ or $\mathbf{b}$ are inclined to the plane of projection, these basis vectors are replaced by $\mathbf{a}_p$ or $\mathbf{b}_p$, respectively.

**Location of origin**: For three-dimensional magnetic space groups, the location of the origin of the two-dimensional magnetic space group symmetry of the projection is given with respect to the unit cell of the three-dimensional magnetic space group. For two-dimensional magnetic space groups, the location of the origin of the one-dimensional magnetic space group symmetry of the projection is given with respect to the unit cell of the two-dimensional magnetic space group.
References


Heesch, H. (1930). Z. fur Kristallogr. 73, 325-345.


Lattices with a first symbol consisting of a single letter with no subscript are lattices of groups $F_1, F_1'$ and $M_1$. To the right of an equality sign, a second symbol gives the generators of the lattice in the subscript of the corresponding lattice symbol. These generating translations are also shown as black arrows in the corresponding figure.

Lattices with a first symbol consisting of a letter with a second letter as a subscript are lattices of magnetic groups $M_R$. The translational subgroup of these groups are of the form $T^M_R = T^D + t_d \cdot T^D$. To the right of equality signs, additional symbols are given which give the generating translations of $T^D$ as a subscript. The translation chosen for $t_d$ is also explicitly given. In the corresponding figures, generating translations which are in $T^D$ are shown in black and generating translations which are in $t_d \cdot T^D$ are shown in red.

### Three-Dimensional Magnetic Lattices:

**Triclinic System**

$$P = P_{a,b,c}$$

**Monoclinic System (2-fold axis along y)**

$$P = P_{a,b,c}$$

$P_{2a} = P_{a,b,2c}$

$t_a = a = (1,0,0)$

$t_b = b = (0,1,0)$

$t_c = c = (0,0,1)$

$P_{2c} = P_{a,b,2c}$

FIGURES 1.1 MAGNETIC SPACE GROUP LATTICES - 1
Orthorhombic System

$P_C = P_{2a,a+b,c} = P_{a-b,a+b,c}$
$\mathbf{t}_u = a = (1,0,0)$

$C = C_{\frac{1}{2}(a+b),b,c}$
$\mathbf{t}_u = c = (0,0,1)$

$C_{2c} = C_{\frac{1}{2}(a+b),b,2c}$
$\mathbf{t}_u = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0)$

$C_P = C_{a+b,b,c} = C_{a,b,c}$

$\mathbf{t}_u = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0)$

$P = P_{a,b,c}$

$P_{2a} = P_{2a,b,c}$
$\mathbf{t}_u = a = (1,0,0)$

$P_{2b} = P_{a,2b,c}$
$\mathbf{t}_u = b = (0,1,0)$

$P_{2c} = P_{a,b,2c}$
$\mathbf{t}_u = c = (0,0,1)$

$P_C = P_{2a,a+b,b,c}$
$\mathbf{t}_u = a = (1,0,0)$

$P_F = P_{2a,a+b,a+c}$
$\mathbf{t}_u = a + b + c = a + b + c$
\[ A = A_{a,b,\frac{1}{2}(b+c)} \]

\[ A_{2a} = A_{2a,b,b+c} \]

\[ t_u = a = (1,0,0) \]

\[ A_p = A_{a,b,c} \]

\[ t_u = \frac{1}{2}(b+c) = (0,\frac{1}{2},\frac{1}{2}) \]

\[ A_i = A_{2a,b,\frac{1}{2}(2a+b+c)} \]

\[ t_u = a = (1,0,0) \]

\[ C = C_{\frac{1}{2}(a+b),b,c} \]

\[ C_{2c} = C_{\frac{1}{2}(a+b),b,2c} \]

\[ t_u = c = (0,0,1) \]

\[ C_p = C_{a+b,b,c} = C_{a,b,c} \]

\[ t_u = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0) \]

\[ C_i = C_{a,b,\frac{1}{2}(a+b+2c)} \]

\[ t_u = c = (0,0,1) \]

\[ F = F_{\frac{1}{2}(a+b),\frac{1}{2}(b+c),\frac{1}{2}(a+c)} \]

\[ F_c = F_{\frac{1}{2}(a+b),b,c} \]

\[ t_u = \frac{1}{2}(a+c) = (\frac{1}{2},0,\frac{1}{2}) \]

\[ F_A = F_{\frac{1}{2}(b+c),c,a} \]

\[ t_u = \frac{1}{2}(a+b) = (\frac{1}{2},\frac{1}{2},0) \]
Tetragonal System

\[ l = l_{a,b,\frac{1}{2}(a+b+c)} \]
\[ l_p = l_{a,b,c} \]
\[ t_u = \frac{1}{2}(a+b+c) = \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) \]
Trigonal System (Rhombohedral Axes)

\[
\mathbf{R} = \mathbf{R}_{a,b,c} \\
\mathbf{R}_{2a,a+b,a+c} = \mathbf{R}_{a+b,b+c,a+c} \\
t_0 = \mathbf{a} = (1,0,0)
\]

Trigonal System (Hexagonal Axes)
Hexagonal System

\[
\mathbf{P} = \mathbf{P}_{a,b,c} \\
\mathbf{P}_{2c} = \mathbf{P}_{a,b,2c} \\
t_0 = \mathbf{c} = (0,0,1)
\]

Cubic System

\[
\mathbf{P} = \mathbf{P}_{a,b,c} \\
\mathbf{P}_F = \mathbf{P}_{2a,a+b,a+c} = \mathbf{P}_{a+b,b+c,a+c} \\
t_0 = \mathbf{a} = (1,0,0)
\]

\[
\mathbf{F} = \mathbf{F}_{\frac{1}{2}(a+b),\frac{1}{2}(b+c),\frac{1}{2}(a+c)}
\]
Two-Dimensional Magnetic Lattices:

Oblique System

\[
\begin{align*}
I &= I_{a,b,\frac{1}{2}(a+b+c)} \\
I_p &= I_{a,b,c} \\
t_a &= \frac{1}{2}(a+b+c) = (\frac{1}{2},\frac{1}{2},\frac{1}{2})
\end{align*}
\]
Rectangular System

- \( p = p_{a,b} \)
- \( p_{2a} = p_{2a,b} \)
- \( t_u = a = (1,0) \)
- \( p_{2b} = p_{a,2b} \)
- \( t_c = b = (0,1) \)
- \( p_c = p_{2a,a+b} = p_{a-b,a+b} \)
- \( t_d = a = (1,0) \)
- \( c = c_{\frac{1}{2}(a+b),b} \)
- \( c_p = c_{a,b} \)
- \( t_d = \frac{1}{2}(a+b) \)
Square System

\[ p = p_{a,b} \]

Hexagonal System

\[ p = p_{a,b} \]

One-Dimensional Magnetic Lattices:

\[ p = p_a \]

\[ p_{2a} = p_{2a} \]

\[ t_u = a = (1) \]
Figures 2.2.3.1: Projection Diagrams of the Three-Dimensional Magnetic Space Groups

Figure 2.2.3.1a: Diagrams for triclinic 3D-magnetic space groups

Figure 2.2.3.1b: Diagrams for monoclinic 3D-magnetic space groups
**Figure 2.2.3.1c**: Diagrams for orthorhombic 3D-magnetic space groups.

**Figure 2.2.3.1d**: Diagrams for tetragonal and cubic 3D-magnetic space groups.
**Figure 2.2.3.1e**: Diagrams for trigonal P and hexagonal 3D-magnetic space groups.

**Figure 2.2.3.1f**: Diagrams for Rhombohedral R 3D-magnetic space groups.
Appendix 1.1: On characterizing a change in coordinate systems and the non-magnetic subgroup of index two of magnetic groups.

When given a subgroup $D$ of index 2 of a group $F$ we want to give enough information to show
1) how to change the origin and
2) how to change the basis vectors of the coordinate system $(O;a,b,c)$ in which $F$ is defined, such in a second coordinate system $(O+t;a',b',c')$ the translational subgroup of $D$ and the set of coset representatives of $D$ with respect to its translational subgroup will be identical with the translational subgroup and standard set of coset representatives of the group of type $D$ listed in the tables. Therefore:

1) We give, in the coordinate system of $F$, the translation $t$ such that the new origin $O+t$ is the origin of the coordinate system in which the subgroup $D$ will be of the form of the representative group $D$ listed in the tables.

2) We give the basis vectors $a',b',c'$ of a coordinate system $(0+t;a',b',c')$ in terms of the basis vectors of the coordinate system in which $F$ is defined, such that the subgroup $D$ in $(0+t;a',b',c')$ is identical with the representative group $D$. 

APPENDIX 1.1 - 1
The lattices of both $F$ and $D$ can be either centered or primitive, consequently:

<table>
<thead>
<tr>
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<th>Primitive $F$</th>
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<tbody>
<tr>
<td>Primitive</td>
<td>$a', b', c'$ of primitive cell of $D$ given in terms of $a, b, c$ of primitive cell of $F$.</td>
</tr>
<tr>
<td>Centered</td>
<td>$a', b', c'$ of conventional unit cell of $D$ given in terms of $a, b, c$ of primitive cell of $F$.</td>
</tr>
<tr>
<td>Primitive $D$</td>
<td>$a', b', c'$ of conventional unit cell of $D$ given in terms of $a, b, c$ of primitive cell of $F$.</td>
</tr>
<tr>
<td>Centered</td>
<td>$a', b', c'$ of conventional unit cell of $D$ given in terms of $a, b, c$ of primitive cell of $F$.</td>
</tr>
</tbody>
</table>

To summarize: For the subgroup $D$ we will give the following symbol:

$$D\left(t; a', b', c'\right)$$

where $D$ is the group type symbol for the group $D$, and $\left(t; a', b', c'\right)$ defines the new coordinate system $(O+t; a', b', c')$ in which the elements of $D$ are identical with those of the representative group of the type $D$. Note that in the tables the symbol $t$ is given by a trio of numbers $n_a, n_b, n_c$ and the translation is defined by

$$t = n_a a + n_b b + n_c c,$$

i.e. the translation $t$ is defined in the coordinate system $(O; a, b, c)$ of the group $F$. The symbol $(O+t; a', b', c')$ is be interpreted to define the new coordinate system by first moving the origin and then inserting the new set of basis vectors at the new origin $O+t$.

The coset representatives of the group $D$ change when changing the origin of
the coordinate system. How they change is as follows:

Given a coordinate system \((\mathbf{O};\mathbf{a},\mathbf{b},\mathbf{c})\) and two points \(\mathbf{x}\) and \(\mathbf{x}'\) in this coordinate system. Given a second coordinate system \((\mathbf{O}+\mathbf{t};\mathbf{a},\mathbf{b},\mathbf{c})\) where the two points corresponding to \(\mathbf{x}\) and \(\mathbf{x}'\) are in the second coordinate system denoted respectively by \(\mathbf{y}\) and \(\mathbf{y}'\).

\[
\begin{align*}
\mathbf{x} &= \mathbf{y} + t \\
\mathbf{x}' &= \mathbf{y}' + t
\end{align*}
\]

If \(\mathbf{x}\) and \(\mathbf{x}'\) are related by \((R|\tau)\), in the first coordinate system, how is this relationship represented in the second coordinate system between \(\mathbf{y}\) and \(\mathbf{y}'\)?

\[
\begin{align*}
\mathbf{x}' &= (R|\tau)\mathbf{x} \\
\mathbf{x}' &= R\mathbf{x} + \tau \\
\mathbf{y}' + t &= R(\mathbf{y} + t) + \tau \\
\mathbf{y}' &= R\mathbf{y} + \tau + R\mathbf{t} - t \\
\mathbf{y}' &= (R|\tau + R\mathbf{t} - t)\mathbf{y} \\
\mathbf{y}' &= (E|-t)(R|\tau)(E|\mathbf{t})\mathbf{y}
\end{align*}
\]

Consequently, when the origin is moved from \(\mathbf{O}\) to \(\mathbf{O}+\mathbf{t}\), the coset \((R|\tau)\) in the first coordinate system \((\mathbf{O};\mathbf{a},\mathbf{b},\mathbf{c})\) becomes, in the second coordinate system \((\mathbf{O}+\mathbf{t};\mathbf{a},\mathbf{b},\mathbf{c})\) the coset \((E|-t)(R|\tau)(E|\mathbf{t}) = (R|\tau + R\mathbf{t} - t)\), i.e. the rotational part remains the same, and \(R\mathbf{t} - \mathbf{t}\) is added to the translational part.
Table 1.1

MAGNETIC SPACE GROUP SYMBOLS AND ELEMENTS

SUPERFAMILIES OF THREE DIMENSIONAL MAGNETIC SPACE GROUPS

HIERARCHAL MAGNETIC SPACE GROUP SUPERFAMILY INDEX

MAGNETIC SPACE GROUP INDEX

SUPERFAMILIES OF TWO-DIMENSIONAL MAGNETIC SPACE GROUPS

SUPERFAMILIES OF ONE-DIMENSIONAL MAGNETIC SPACE GROUPS
<table>
<thead>
<tr>
<th>System</th>
<th>Symbol</th>
<th>Symbol</th>
<th>Symbol</th>
<th>Symbol</th>
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</thead>
<tbody>
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<td>P1</td>
<td>P2&amp;</td>
<td>P2</td>
<td>C2</td>
</tr>
<tr>
<td></td>
<td>P2/m</td>
<td>P21/m</td>
<td>C2/m</td>
<td>P2/c</td>
</tr>
<tr>
<td></td>
<td>P2/c</td>
<td>P21/c</td>
<td>C2/c</td>
<td></td>
</tr>
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<td>Orthorhombic</td>
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<td>P222_2</td>
<td>P222_3</td>
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<td></td>
<td></td>
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<td>P222_2</td>
<td>P222_3</td>
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<td>P222_2</td>
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<tr>
<td>Tetragonal</td>
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<td>P4_1</td>
<td>P4_2</td>
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<td>P4_n</td>
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ORTHORHOMBIC SYSTEM

**16.1.99** P222

20.2.123 C222,1'
| 22.4.143 | Fc 222 | 25.13.167 | Pa mm'2 | 28.7.191 | P2c ma2 |
| 22.5.144 | Fc 22'2' | | | | |
| 23.1.145 | I222 | 26.1.168 | Pmc2 | 28.1.193 | P2b ma2 |
| 23.2.146 | I2221' | 26.2.169 | Pmc2,1' | 28.9.194 | P2c m'a2 |
| 23.3.147 | I2'2'2 | 26.3.170 | Pm'c2',1 | 28.11.195 | P2c ma2 |
| 23.4.148 | Ip 222 | 26.4.171 | Pm'c2',1 | 28.12.196 | P2c m'a2 |
| 23.5.149 | Ip 2'2'2 | 26.5.172 | Pm'c2',1 | 28.13.197 | P'A ma2 |
| 24.1.150 | I2,2,2,1 | 26.6.174 | P2b mc2,1 | 29.1.198 | Pca2 |
| 24.2.151 | I2,2,2,1,1' | 26.7.175 | Pc mc2,1 | 29.2.199 | Pca2,1' |
| 24.3.152 | I2',2',2,1 | 26.8.176 | P2a mc2',1 | 29.3.200 | P'a2,1' |
| 24.4.153 | Ip 2',2',2,1 | 26.9.177 | P2b m'c2',1 | 29.4.201 | Pca2,1' |
| 24.5.154 | Ip 2',2',2,1 | 27.1.178 | Pcc2 | 29.5.202 | P'a2,1' |
| 25.1.155 | Pmm2 | 27.2.179 | Pcc2,1 | 29.6.203 | P2b c'a2,1 |
| 25.2.156 | Pmm21' | 27.3.180 | Pc'c2' | 29.7.204 | P2b c'a2,1 |
| 25.3.157 | Pm'm2' | 27.4.181 | Pc'c'2' | 30.1.205 | Pnc2 |
| 25.4.158 | Pm'm2 | 27.5.182 | P2a cc2 | 30.2.206 | Pnc2,1 |
| 25.5.159 | P2c mm2 | 27.6.183 | Pc cc2 | 30.3.207 | Pnc2' |
| 26.6.160 | P2a mm2 | 27.7.184 | P2b c'c2' | 30.4.208 | Pnc2' |
| 26.7.161 | Pc mm2 | 28.1.185 | Pma2 | 30.5.209 | Pn'c2' |
| 25.8.162 | Pa mm2 | 28.2.186 | Pma2,1' | 30.6.210 | P2a nc2 |
| 25.9.163 | Pf mm2 | 28.3.187 | Pm'a2' | 30.7.211 | P2a nc2,1' |
| 25.10.164 | P2c mm2 | 28.4.188 | Pma'2' | 31.1.212 | Pmn2,1' |
| 25.11.165 | P2c m'm2' | 28.5.189 | Pma'2 | 31.2.213 | Pmn2,1' |
| 25.12.166 | P2a m'm2 | 28.6.190 | P2b ma2 | 31.3.214 | Pmn2,1' |
31.4.215 Pmn'2, 35.4.239 Cm'm'2 37.7.264 C_p c'c'2
31.5.216 Pm'n'2 35.5.240 C_{2c} mm2
31.6.217 P_2{\alpha} mn2, 35.6.241 C_p mm2 38.1.265 Amm2
31.7.218 P_2{\alpha} m'n2, 35.7.242 C_{1} mm2 38.2.266 Amm21'
32.1.219 Pba2 35.8.243 C_{2c} m'm'2 38.4.268 Amm'2'
32.2.220 Pba21' 35.9.244 C_{2c} m'm'2 38.5.269 Am'm'2
32.3.221 Pb'a2' 35.10.245 C_p m'm'2 38.6.270 A_{2a} mm2
32.4.222 Pb'a2 35.11.246 C_{1} m'm'2 38.7.271 A_{p} mm2
32.5.223 P_2{\alpha} ba2 35.12.247 C_{1} m'm'2 38.8.272 A_{1} mm2
32.6.224 P_2{\alpha} b'a2' 35.13.248 C_{1} m'm'2 38.9.273 A_{2a} mm'2'
32.7.225 P_2{\alpha} b'a2 36.1.249 Cm'c2 39.10.274 A_{p} m'm'2
33.1.226 Pna2 36.2.250 Cm'c2,1' 38.11.275 A_{p} mm'2'
33.2.227 Pna2,1' 36.3.251 Cm'c2,1' 38.12.276 A_{p} m'm'2
33.3.228 Pn'a2,1' 36.4.252 Cm'c2,1' 38.13.277 A_{1} m'm'2
33.4.229 Pn'a2,1' 36.5.253 Cm'c2,1' 39.1.278 Abm2
33.5.230 Pn'a2 36.6.254 C_p mc2,1 39.2.279 Abm21'
34.1.231 Pnn2 36.7.255 C_p m'c2,1' 39.3.280 Ab'm'2
34.2.232 Pnn21' 36.8.256 C_p m'c2,1' 39.4.281 Ab'm'2
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34.4.234 Pn'n2 37.2.259 Ccc2,1' 39.6.283 A_{2a} bm2
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35.2.237 Cmm21' 37.5.262 C_{p} cc2 39.9.286 A_{2a} b'm'2
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137.7.1167 P42'/nm'c' 139.14.1192 I_p,4'/m'm'm 141.5.1217 I4, /'am'd
137.8.1168 P42'/n'mc' 139.15.1193 I_p,4'/mmm'm 141.6.1218 I4, /a'm'd
137.9.1169 P42'/n'm'c' 139.16.1194 I_p,4'/m'm'm 141.7.1219 I4, /am'd
138.1.1170 P42'/ncm 139.17.1195 I_p,4'/m'm'm 141.8.1220 I4, /'a'm'd
138.2.1171 P42'/ncm1' 140.1.1196 I4/mcm 141.9.1221 I4, /a'm'd'
138.3.1172 P42'/nc'm 140.2.1197 I4/mcm1' 142.1.1222 I4, /acd
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138.6.1175 P42'/n'c'm 140.5.1200 I4'/mcm' 142.4.1225 I4, /'ac'd
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138.8.1177 P42'/n'c'm' 140.7.1202 I4/mc'm' 142.6.1227 I4, /'a'c'd
138.9.1178 P42'/n'c'c'm' 140.8.1203 I4'/m'c'm' 142.7.1228 I4, /ac'd'
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139.3.1181 I4/m'cm 140.11.1206 I_p,4/m'c'm 142.10.1231 P3
139.4.1182 I4'/m'm'm 140.12.1207 I_p,4'/mc'm 143.1.1232 P31'
139.5.1183 I4'/mmm'm 140.13.1208 I_p,4'/mcm' 143.2.1233 P_3c 3
139.6.1184 I4'/m'm'm 140.14.1209 I_p,4'/m'c'm 143.3.1233 P_3c 3
139.7.1185 I4/m'm'm 140.15.1210 I_p,4/mc'm 143.4.1234 P_3 3_1
139.8.1186 I4'/m'm'm 140.16.1211 I_p,4'/m'c'm 144.1.1235 P_3 3_1'
139.9.1187 I4/m'm'm 140.17.1212 I_p,4/m'c'm' 144.2.1236 P_3 3_2
139.10.1188 I_p,4/mmm 141.1.1213 I4/, /amd 144.3.1237 P_3 3_2
139.11.1189 I_p,4/m'mm
HEXAGONAL SYSTEM
188.1.1446  P\&c2
188.2.1447  P\&c21'
188.3.1448  P\&'c'2
188.4.1449  P\&'c'2'
188.5.1450  P\&c'2'

189.1.1451  P\&2m
189.2.1452  P\&2m1'
189.3.1453  P\&'2'm
189.4.1454  P\&'2'm'
189.5.1455  P\&2'm'
189.6.1456  P\&2'm 192.1.1476  P6/mcc
189.7.1457  P\&2'm'

190.1.1458  P\&2c
190.2.1459  P\&2c1'
190.3.1460  P\&'2'c
190.4.1461  P\&'2'c'
190.5.1462  P\&2'c'

191.1.1463  P6/mmm
191.2.1464  P6/mmm1'
191.3.1465  P6/m'mm
191.4.1466  P6'/m'mm
191.5.1467  P6'/mmm'
191.6.1468  P6'/m'm'm
191.7.1469  P6'/m'm'm'

194.1.1494  P6_3/mmc
194.2.1495  P6_3/mmc1'
194.3.1496  P6_3/m'mc
194.4.1497  P6_3/m'mc'
194.5.1498  P6_3/mmc'
194.6.1499  P6_3/m'mc
194.7.1500  P6_3/m'mc'
194.8.1501  P6_3/m'mc'
194.9.1502  P6_3/m'mc'

CUBIC SYSTEM

195.1.1503  P23
195.2.1504  P231'
195.3.1505  P F23
195.4.1506  F23
195.5.1507  F231'
196.2.1508  I23
196.3.1509  I231'
197.3.1510  I_{p}23
197.4.1511  P2_3
198.2.1512  P2_31'
199.2.1513  I_{2,3}
199.3.1514  I_{2,3}1'
199.4.1515  I_{p}2_3
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218.2.1586  P43n1' 223.4.1609  Pm3'n 227.5.1632  Fd3'3'm'
218.3.1587  P4'3'n 223.5.1610  Pm3'n 228.1633  Fd3c

219.1.1588  F43c  224.1.1611  Pn3m  228.2.1634  Fd3c1'
219.2.1589  F43c1'  224.2.1612  Pn3m1'  228.3.1635  Fd3c'
219.3.1590  F4'3c'  224.3.1613  Pn3'm  228.4.1636  Fd3c'
220.1.1591  I43d  224.4.1614  Pn3'm  228.5.1637  Fd3c'
220.2.1592  I43d1'  224.5.1615  Pn3'm'  229.1.1638  Im3m
220.3.1593  I4'3d'  224.6.1616  Pf3m  229.2.1639  Im3m1'
221.1.1594  Pm3m  224.7.1617  Pf3m'  229.3.1640  Im3'm
221.2.1595  Pm3m1'  225.1.1618  Fm3m  229.4.1641  Im3'm
221.3.1596  Pm3'm  225.2.1619  Fm3m1'  229.5.1642  Im3'm'
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221.6.1599  Pf3m3m  225.5.1622  Fm3'm'  229.8.1645  Ip3m3'm'
221.7.1600  Pf3m3m' 226.1.1623  Fm3c

222.1.1601  Pn3n  226.2.1624  Fm3c1'  230.1.1647  Ia3d
222.2.1602  Pn3n1'  226.3.1625  Fm3c'  230.2.1648  Ia3d1'
222.3.1603  Pn3'n  226.4.1626  Fm3c'  230.3.1649  Ia3'd
222.4.1604  Pn3'n  226.5.1627  Fm3c'  230.4.1650  Ia3'd'
222.5.1605  Pn3'n  227.1.1628  Fd3m
223.1.1606  Pm3n  227.2.1629  Fd3m1'
### TRICLINIC SYSTEM

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### MONOCLINIC SYSTEM

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<td>P&lt;sub&gt;2a&lt;/sub&gt; &amp; c</td>
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<td>7.6.37</td>
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<td>8.1.38</td>
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<td>8.2.39</td>
<td>Cm&lt;sup&gt;1′&lt;/sup&gt;</td>
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<td>8.3.40</td>
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<td>P2$_2$/m</td>
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<td>13.8.84</td>
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<td>14.2.87</td>
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<td>14.4.89</td>
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<td>14.5.90</td>
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<td>14.6.91</td>
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<td>P2_1/c</td>
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<td>15.7.98</td>
<td>C_p 2'/c</td>
<td>P2_1/c</td>
<td>(1/4,1/4,0;a,b,c)</td>
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**ORTHORHOMBIC SYSTEM**

<p>| 16.1.99  | P222       | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_z</em>0,0,0) |
| 16.2.100 | P2221'     |           |               |           |               |
| 16.3.101 | P2'2'2     | P2        | (0,0,0;b,c,a) | (1<em>0,0,0) | (2_x</em>0,0,0)' | (2,<em>0,0,0)' | (2_z</em>0,0,0) |
| 16.4.102 | P_2a 222   | P222      | (0,0,0;2a,b,c) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_x</em>0,0,0) |
| 16.5.103 | P_c 222    | C222      | (0,0,0;2a,2b,c) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_x</em>0,0,0) |
| 16.6.104 | P_f 222    | F222      | (0,0,0;2a,2b,2c) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_x</em>0,0,0) |
| 16.7.105 | P_2c 22'2' | P222_1    | (0,0,0;a,b,2c) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,1) | (2_x</em>0,0,1) |</p>
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<th>(2ₓ*0,0,0)</th>
<th>(2ᵧ*0,0,1/2)</th>
<th>(2ᶻ*0,0,1/2)</th>
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<td>17.3.108</td>
<td>P₂'₂'₂₁ P₂₁</td>
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<td>(1*0,0,0)</td>
<td>(2ₓ*0,0,0)'</td>
<td>(2ᵧ*0,0,1/2)'</td>
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<td>(2ᵧ*0,0,1/2)'</td>
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<td>(2ₓ*0,0,0)</td>
<td>(2ᵧ*0,0,1/2)</td>
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<td>17.7.112</td>
<td>P₂₂₂'²₂₁ P₂₁₂₂</td>
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<td>18.3.115</td>
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<td>(2ᵧ*1/2,1/2,0)'</td>
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MAGNETIC SPACE GROUP ELEMENTS 8
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<td>19.3.121</td>
<td>$P_{212121}$  $P_{21}$  $(1/4,0,0;b,c,a)$  $(1<em>0,0,0)$  $(2_x</em>1/2,1/2,0)'$  $(2_y<em>0,1/2,1/2)'$  $(2_z</em>1/2,0,1/2)$</td>
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<td>20.1.122</td>
<td>$C_{222_1}$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)$  $(2_y<em>0,0,1/2)$  $(2_z</em>0,0,1/2)$</td>
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<td>$C_{222_1}'$</td>
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<td>20.3.124</td>
<td>$C_{2'2'2_1}$  $P_{21}$  $(0,0,0;b,c,(a+b)/2)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)'$  $(2_y<em>0,0,1/2)'$  $(2_z</em>0,0,1/2)'$</td>
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<td>20.4.125</td>
<td>$C_{2'2_1'}$  $P_{2}$  $(0,0,0;c,a,(a+b)/2)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)$  $(2_y<em>0,0,1/2)'$  $(2_z</em>0,0,1/2)'$</td>
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<td>20.5.126</td>
<td>$C_{p_{222_1}}$  $P_{222_1}$  $(0,0,0;a,b,c)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)$  $(2_y<em>0,0,1/2)$  $(2_z</em>0,0,1/2)$</td>
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<td>20.6.127</td>
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<td>20.7.128</td>
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<td>21.3.131</td>
<td>$C_{2'2'2}$  $P_{2}$  $(0,0,0;b,c,(a+b)/2)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)'$  $(2_y<em>0,0,0)'$  $(2_z</em>0,0,0)$</td>
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<tr>
<td>21.4.132</td>
<td>$C_{2'2'}$  $C_{2}$  $(0,0,0;\delta,a,c)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)$  $(2_y<em>0,0,0)'$  $(2_z</em>0,0,0)'$</td>
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<tr>
<td>21.5.133</td>
<td>$C_{2c_{222}}$  $C_{222}$  $(0,0,0;a,b,2c)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)$  $(2_y<em>0,0,0)$  $(2_z</em>0,0,0)$</td>
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<tr>
<td>21.6.134</td>
<td>$C_{p_{222}}$  $P_{222}$  $(0,0,0;a,b,c)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)$  $(2_y<em>0,0,0)$  $(2_z</em>0,0,0)$</td>
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<tr>
<td>21.7.135</td>
<td>$C_{i_{222}}$  $I_{222}$  $(0,0,0;a,b,2c)$  $(1<em>0,0,0)$  $(2_x</em>0,0,0)$  $(2_y<em>0,0,0)$  $(2_z</em>0,0,0)$</td>
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**MAGNETIC SPACE GROUP ELEMENTS 9**
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<th>Number</th>
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<th>Equations</th>
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<tr>
<td>21.8.136</td>
<td>C\textsubscript{2\textgamma} 2\textgamma'2'</td>
<td>C\textsubscript{222\textsubscript{1}}</td>
<td>(0,0,0; a,b,2c) (1\textbullet<em>0,0,0) (2\textbullet</em>0,0,0) (2\textbullet<em>0,0,1) (2\textbullet</em>0,0,1)</td>
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<tr>
<td>21.9.137</td>
<td>C\textsubscript{\textgamma} 2\textgamma'2'</td>
<td>P\textsubscript{2\textgamma,2\textgamma}</td>
<td>(0,0,0; a,b,c) (1\textbullet<em>0,0,0) (2\textbullet</em>0/1,1/2,0) (2\textbullet<em>0/1,1/2,0) (2\textbullet</em>0,0,0)</td>
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<tr>
<td>21.10.138</td>
<td>C\textsubscript{\textgamma} 2\textgamma'2'</td>
<td>P\textsubscript{2\textgamma2\textsubscript{1}}</td>
<td>(1/4,0,0; a,&amp; b) (1\textbullet<em>0,0,0) (2\textbullet</em>0,0,0) (2\textbullet<em>0,1/2,1/2) (2\textbullet</em>0,1/2,1/2)</td>
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<tr>
<td>21.11.139</td>
<td>C\textsubscript{2\textgamma}2\textgamma'2'</td>
<td>I\textsubscript{2,2,2\textsubscript{1}}</td>
<td>(1/4,0,0; a,b,2c) (1\textbullet<em>0,0,0) (2\textbullet</em>0,0,1) (2\textbullet<em>0,0,0) (2\textbullet</em>0,0,1)</td>
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<tr>
<td>22.1.140</td>
<td>F2\textgamma2\textgamma</td>
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<tr>
<td>22.2.141</td>
<td>F2\textgamma2\textgamma1'</td>
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<tr>
<td>22.3.142</td>
<td>F2'2'2'</td>
<td>C\textsubscript{2}</td>
<td>(0,0,0; b,c,{a+b}/2) (1\textbullet<em>0,0,0) (2\textbullet</em>0,0,0)' (2\textbullet<em>0,0,0)' (2\textbullet</em>0,0,0)</td>
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<td>22.4.143</td>
<td>F\textsubscript{c} 2\textgamma2\textgamma</td>
<td>C\textsubscript{222}</td>
<td>(0,0,0; a,b,c) (1\textbullet<em>0,0,0) (2\textbullet</em>0,0,0) (2\textbullet<em>0,0,0) (2\textbullet</em>0,0,0)</td>
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<td>22.5.144</td>
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<td>(0,0,0; a+b,c,a) (1\textbullet<em>0,0,0) (2\textbullet</em>0,0,0)' (2\textbullet<em>0,0,0)' (2\textbullet</em>0,0,0)</td>
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<td>(2z*1/2,1/2,0)</td>
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<td>(2z*0,0,1/2)</td>
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<td>Abm2</td>
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<td><strong>26.1.168</strong></td>
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<td>26.4.171</td>
<td>$Pmc'_{21}'$</td>
<td>Pm</td>
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<td>Pmc$_2$</td>
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<td>26.7.174</td>
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<td>Pmc$_2$</td>
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<td>26.8.175</td>
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<td>Cmc$_2$</td>
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<td>26.9.176</td>
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<td>Pmn$_2$</td>
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<td>26.10.177</td>
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<td><strong>27.1.178</strong></td>
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<td>Pc</td>
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<td>P2</td>
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<td>27.5.182</td>
<td>$P_{2a}cc_{2}$</td>
<td>Pcc$_2$</td>
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<td>P\textsubscript{c} cc2</td>
<td>Ccc2</td>
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<td>27.7.184</td>
<td>P\textsubscript{2}b c'c2'</td>
<td>Pnc2</td>
<td>(0,1/2,0;a,2b,c)</td>
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</table>

<p>| 28.1.185 | Pma2 | | (1*0,0,0) | (m\textsubscript{x}*1/2,0,0) | (m\textsubscript{y}*1/2,0,0) | (2\textsubscript{z}<em>0,0,0) |
| 28.2.186 | Pma2' | | | | | |
| 28.3.187 | Pm'a2' | P\textsubscript{c} | (0,0,0;c,6;a) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,0)' | (m\textsubscript{y}*1/2,0,0) | (2\textsubscript{z}<em>0,0,0)' |
| 28.4.188 | Pma'2' | P\textsubscript{m} | (1/4,0,0;c,a,b) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,0) | (m\textsubscript{y}*1/2,0,0)' | (2\textsubscript{z}<em>0,0,0)' |
| 28.5.189 | Pm'a2' | P\textsubscript{2} | (0,0,0;b,c,a) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,0)' | (m\textsubscript{y}*1/2,0,0)' | (2\textsubscript{z}<em>0,0,0) |
| 28.6.190 | P\textsubscript{2}b ma2 | Pma2 | (0,0,0;a,2b,c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,0) | (m\textsubscript{y}*1/2,0,0) | (2\textsubscript{z}<em>0,0,0) |
| 28.7.191 | P\textsubscript{2}c ma2 | Pma2 | (0,0,0;a,b,2c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,0) | (m\textsubscript{y}*1/2,0,0) | (2\textsubscript{z}<em>0,0,0) |
| 28.8.192 | P\textsubscript{A} ma2 | Ama2 | (0,0,0;a,2b,2c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,0) | (m\textsubscript{y}*1/2,0,0) | (2\textsubscript{z}<em>0,0,0) |
| 28.9.193 | P\textsubscript{2}b m'a2' | P\textsubscript{ba2} | (0,1/2,0;a,2b,c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,1,0) | (m\textsubscript{y}*1/2,0,0) | (2\textsubscript{z}<em>0,1,0) |
| 28.10.194 | P\textsubscript{2}c m'a2' | P\textsubscript{ca2} | (0,0,0;a,b,2c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,1) | (m\textsubscript{y}*1/2,0,0) | (2\textsubscript{z}<em>0,0,1) |
| 28.11.195 | P\textsubscript{2}c ma'2' | Pmn2\textsubscript{1} | (1/4,0,0;a,b,2c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,0) | (m\textsubscript{y}*1/2,0,1) | (2\textsubscript{z}<em>0,0,1) |
| 28.12.196 | P\textsubscript{2}c m'a'2 | Pnc2 | (0,0,0;b,6;2c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,0,1) | (m\textsubscript{y}*1/2,0,1) | (2\textsubscript{z}<em>0,0,0) |
| 28.13.197 | P\textsubscript{A} m'a'2 | A\textsubscript{ba2} | (0,0,0;a,2b,2c) | (1</em>0,0,0) | (m\textsubscript{x}*1/2,1,0) | (m\textsubscript{y}*1/2,1,0) | (2\textsubscript{z}*0,0,0) |
| 29.1.198 | Pca2 (<em>1) | (1(\ast)0,0,0) | ((m_x)(\ast)1/2,0,1/2) | ((m_y)(\ast)1/2,0,0) | (2(\ast)0,0,1/2) |
| 29.2.199 | Pca2(</em>{1'}) |
| 29.3.200 | Pc'a2 (_1)' (Pc) | (0,0,0;c,(\varepsilon),a) | (1(\ast)0,0,0) | ((m_x)(\ast)1/2,0,1/2)' | ((m_y)(\ast)1/2,0,0) | (2(\ast)0,0,1/2)' |
| 29.4.201 | Pca'2 (_1)' (Pc) | (1/4,0,0;b,(\varepsilon),c) | (1(\ast)0,0,0) | ((m_x)(\ast)1/2,0,1/2) | ((m_y)(\ast)1/2,0,0)' | (2(\ast)0,0,1/2)' |
| 29.5.202 | Pc'a2 (<em>1) (P2_1) | (0,0,0;b,c,a) | (1(\ast)0,0,0) | ((m_x)(\ast)1/2,0,1/2)' | ((m_y)(\ast)1/2,0,0)' | (2(\ast)0,0,1/2) |
| 29.6.203 | P(</em>{2b}) ca2 (_1) (Pca2(<em>1)) | (0,0,0;a,2b,c) | (1(\ast)0,0,0) | ((m_x)(\ast)1/2,0,1/2) | ((m_y)(\ast)1/2,0,0) | (2(\ast)0,0,1/2) |
| 29.7.204 | P(</em>{2b}) c'a2 (_1) (Pna2(<em>1)) | (0,0,0;a,2b,c) | (1(\ast)0,0,0) | ((m_x)(\ast)1/2,1,1/2) | ((m_y)(\ast)1/2,1,0) | (2(\ast)0,0,1/2) |
| 30.1.205 | Pnc2 | (1(\ast)0,0,0) | ((m_x)(\ast)0,1/2,1/2) | ((m_y)(\ast)0,1/2,1/2) | (2(\ast)0,0,0) |
| 30.2.206 | Pnc2(<em>1)' |
| 30.3.207 | Pn'c2' (Pc) | (0,1/4,0;a,b,c) | (1(\ast)0,0,0) | ((m_x)(\ast)0,1/2,1/2)' | ((m_y)(\ast)0,1/2,1/2) | (2(\ast)0,0,0)' |
| 30.4.208 | Pnc2' (Pc) | (0,0,0;c,a,b+c) | (1(\ast)0,0,0) | ((m_x)(\ast)0,1/2,1/2) | ((m_y)(\ast)0,1/2,1/2)' | (2(\ast)0,0,0)' |
| 30.5.209 | Pn'c2' (P2) | (0,0,0;b,c,a) | (1(\ast)0,0,0) | ((m_x)(\ast)0,1/2,1/2)' | ((m_y)(\ast)0,1/2,1/2)' | (2(\ast)0,0,0) |
| 30.6.210 | P(</em>{2a}) hc2 (Pnc2) | (0,0,0;2a,b,c) | (1(\ast)0,0,0) | ((m_x)(\ast)0,1/2,1/2) | ((m_y)(\ast)0,1/2,1/2) | (2(\ast)0,0,0) |
| 30.7.211 | P(</em>{2a}) nc2' (Pnn2) | (1/2,0,0;2a,b,c) | (1(\ast)0,0,0) | ((m_x)(\ast)0,1/2,1/2) | ((m_y)(\ast)1/2,1/2) | (2(\ast)1,0,0) |
| 31.1.212 | Pmn2 (_1) | (1(\ast)0,0,0) | ((m_x)(\ast)0,0,0) | ((m_y)(\ast)1/2,0,1/2) | (2(\ast)1/2,0,1/2) |</p>
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<th>Description</th>
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<td>(1*0,0,0)</td>
<td>((m_x*0,0,0)')</td>
<td>((m_y*1/2,0,1/2))</td>
<td>((2_z*1/2,0,1/2))'</td>
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<tr>
<td>Pm'n2₃</td>
<td>((0,0,0;b,\delta, c))</td>
<td>(1*0,0,0)</td>
<td>((m_x*0,0,0))</td>
<td>((m_y*1/2,0,1/2))'</td>
<td>((2_z*1/2,0,1/2))'</td>
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<td>Pmn'2₃</td>
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<td>(1*0,0,0)</td>
<td>((m_x*0,0,0)')</td>
<td>((m_y*1/2,0,1/2))'</td>
<td>((2_z*1/2,0,1/2))'</td>
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<tr>
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<td>((0,0,0;b,2b, c))</td>
<td>(1*0,0,0)</td>
<td>((m_x*0,0,0))</td>
<td>((m_y*1/2,0,1/2))</td>
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<td>Pb'a₂</td>
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<tr>
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<td>Pba₂</td>
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<td>Pmc₂₁</td>
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| 37.3.260    | Cc'c₂'     | Cc      | (0,0,0;a,b,c) | (1*0,0,0) | (mₓ*0,0,1/2)' | (mᵧ*0,0,1/2) | (2*₀,0,0)'}
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<th>Symbol Interpretation</th>
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<td>A2b'm2'</td>
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<td>(0,1/4,0;b,c,a)</td>
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<td>(m_x*0,0,1/2)</td>
<td>(m_y*0,1/2,0)</td>
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<td>Pca2_1</td>
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<td>39.12.289</td>
<td>A2b'm2'</td>
<td>Pcc2</td>
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<td>(m_y*0,0,1/2)</td>
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<tr>
<td>39.13.290</td>
<td>A2b'm2'</td>
<td>Iba2</td>
<td>(0,0,0;2a,b,c)</td>
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<td>(m_y*1,1/2,0)</td>
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<td>40.1.291</td>
<td>Ama2</td>
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<td>(m_y*1/2,0,0)</td>
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<td>40.2.292</td>
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<td>40.3.293</td>
<td>Am'a2'</td>
<td>Cc</td>
<td>(0,0,0;c,b,a)</td>
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<td>(m_y*1/2,0,0)</td>
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MAGNETIC SPACE GROUP ELEMENTS 19
40.4.294  Ama'2'  Pm  (1/4,0,0;b,\&c,(b+c)/2)  (1*0,0,0)  (m_x*1/2,0,0)  (m_y*1/2,0,0)'  (2_z*0,0,0)'
40.5.295  Am'a2  C2  (0,0,0;b,c,a)  (1*0,0,0)  (m_x*1/2,0,0)'  (m_y*1/2,0,0)'  (2_z*0,0,0)
40.6.296  A_p ma2  Pma2  (0,0,0;a,b,c)  (1*0,0,0)  (m_x*1/2,0,0)  (m_y*1/2,0,0)  (2*z*0,0,0)
40.7.297  A_p ma2'  Pnma2  (0,0,0;\{b+c\},a,b)  (1*0,0,0)  (m_x*1/2,0,0)  (m_y*1/2,0,0)  (2*z*0,0,0)
40.8.298  A_p ma2'  Pmn2  (1/4,1/4,0;a,b,c)  (1*0,0,0)  (m_x*1/2,0,0)  (m_y*1/2,0,0)  (2*z*0,0,0)
40.9.299  A_p ma2'  Pnn2  (0,0,0;a,b,c)  (1*0,0,0)  (m_x*1/2,0,0)  (m_y*1/2,0,0)  (2*z*0,0,0)

41.1.300  Aba2  (1*0,0,0)  (m_x*1/2,1/2,0)  (m_y*1/2,1/2,0)  (2*z*0,0,0)
41.2.301  Aba21'
41.3.302  Ab'a2  Cc  (0,1/4,0;c,\&d,a)  (1*0,0,0)  (m_x*1/2,1/2,0)'  (m_y*1/2,1/2,0)  (2*z*0,0,0)'
41.4.303  Aba'2'  Pd  (1/4,0,0;\{b+c\}/2,a,b)  (1*0,0,0)  (m_x*1/2,1/2,0)  (m_y*1/2,1/2,0)'  (2*z*0,0,0)'
41.5.304  Ab'a2  C2  (0,0,0;b,c,a)  (1*0,0,0)  (m_x*1/2,1/2,0)'  (m_y*1/2,1/2,0)'  (2*z*0,0,0)
41.6.305  A_p ba2  Pba2  (0,0,0;a,b,c)  (1*0,0,0)  (m_x*1/2,1/2,0)  (m_y*1/2,1/2,0)  (2*z*0,0,0)
41.7.306  A_p b'a2'  Pca2  (0,1/4,0;\{b+a\},\&c)  (1*0,0,0)  (m_x*1/2,0,1/2)  (m_y*1/2,0,1/2)  (2*z*0,1/2,1/2)
41.8.307  A_p ba'2'  Pna2  (0,1/4,0;\&b,c)  (1*0,0,0)  (m_x*1/2,0,1/2)  (m_y*1/2,0,1/2)  (2*z*0,1/2,1/2)
41.9.308  A_p b'a2'  Pnc2  (0,0,0;b,\&c)  (1*0,0,0)  (m_x*1/2,0,1/2)  (m_y*1/2,0,1/2)  (2*z*0,0,0)

42.1.309  Fmm2  (1*0,0,0)  (m_x*0,0,0)  (m_y*0,0,0)  (2*z*0,0,0)
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<th>Description</th>
<th>Matrix Elements</th>
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<td>42.3.311 F'm2' Cm</td>
<td>(0,0,0; a, b, (a+c)/2)</td>
<td>(m_x*0,0,0)</td>
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<td>42.4.312 F'm2' C2</td>
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<td>42.5.313 F_c mm2 Cmm2</td>
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<td>(1*0,0,0)</td>
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<td>42.6.314 F_A mm2 Amm2</td>
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<td>(1*0,0,0)</td>
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<td>42.7.315 F_c mm'2 Cmc2'</td>
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<tr>
<td>42.8.316 F_c m'm2' Ccc2'</td>
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<td>42.9.317 F_A m'm2' Abm2</td>
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<td>43.1.320 Fdd2</td>
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<tr>
<td>43.2.321 Fdd2'</td>
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<td>43.3.322 F'd'2' Cc</td>
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<td>43.4.323 F'd'2' C2</td>
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<td>44.1.324 Imm2</td>
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<td>(m_x*0,0,0)</td>
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<td>Pnn2</td>
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<td>Pcc2</td>
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<td>Pca2'</td>
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<td>45.7.337</td>
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<td>46.4.341</td>
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<td>Cm</td>
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MAGNETIC SPACE GROUP ELEMENTS 22
<p>| 46.5.342 | Im'a'2 | C2 | (0,0,0;a+b,c,a) | (1<em>0,0,0) | (m_x</em>1/2,0,0)' | (m_y<em>1/2,0,0)' | (2_z</em>0,0,0) |
| 46.6.343 | I_p ma2 | Pma2 | (0,0,0;a,b,c) | (1<em>0,0,0) | (m_x</em>1/2,0,0) | (m_y<em>1/2,0,0) | (2_z</em>0,0,0) |
| 46.7.344 | I_p ma2' | Pna2 | (1/4,1/4,0;a,b,c) | (1<em>0,0,0) | (m_x</em>0,1/2,1/2) | (m_y<em>1/2,0,0) | (2_z</em>1/2,1/2) |
| 46.8.345 | I_p ma2'' | Pmc2 | (1/4,1/4,0;a,b,c) | (1<em>0,0,0) | (m_x</em>1/2,0,0) | (m_y<em>0,1/2,1/2) | (2_z</em>1/2,1/2) |
| 46.9.346 | I_p ma2' | Pnc2 | (0,0,0;a,b,c) | (1<em>0,0,0) | (m_x</em>1/2,1/2) | (m_y<em>0,1/2,1/2) | (2_z</em>0,0,0) |
| 47.1.347 | Pmmm | | | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_z</em>0,0,0) |
| 47.2.348 | Pmmm1' | | | | | | |
| 47.3.349 | Pm'mm | Pmm2 | (0,0,0;b,c,a) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0)' | (2_z</em>0,0,0)' |
| 47.4.350 | Pm'm'm | P2/m | (0,0,0;b,c,a) | (1<em>0,0,0) | (2_x</em>0,0,0)' | (2_y<em>0,0,0)' | (2_z</em>0,0,0)' |
| 47.5.351 | Pm'm'm' | P222 | (0,0,0;a,b,c) | (1<em>0,0,0) | (2_x</em>0,0,0)' | (2_y<em>0,0,0)' | (2_z</em>0,0,0)' |
| 47.6.352 | P_{2a}mmm | Pmmm | (0,0,0;2a,b,c) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_z</em>0,0,0) |
| 47.7.353 | P_cmmm | Cmmm | (0,0,0;2a,2b,c) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_z</em>0,0,0) |
| 47.8.354 | P_fmmm | Fmmm | (0,0,0;2a,2b,2c) | (1<em>0,0,0) | (2_x</em>0,0,0) | (2_y<em>0,0,0) | (2_z</em>0,0,0) |
| 47.9.355 | P\textsubscript{2}a mmm' | Pmma | ((1/2,0,0;2a,b,c)) | (1*0,0,0) | (2\textsubscript{x} *1,0,0) | (2\textsubscript{y} *1,0,0) | (2\textsubscript{z} <em>0,0,0) |
| 47.10.356 | P\textsubscript{2c} m'm'm | Pccm | ((0,0,0;a,b,2c)) | (1</em>0,0,0) | (2\textsubscript{x} *0,0,1) | (2\textsubscript{y} *0,0,1) | (2\textsubscript{z} <em>0,0,0) |
| 47.11.357 | P\textsubscript{c} mmm' | Cmma | ((1/2,0,0;2b,2&amp;i,c)) | (1</em>0,0,0) | (2\textsubscript{x} *1,0,0) | (2\textsubscript{y} *1,0,0) | (2\textsubscript{z} <em>0,0,0) |
| 48.1.358 | Pnnn | () | () | (1</em>0,0,0) | (2\textsubscript{x} *0,0,0) | (2\textsubscript{y} *0,0,0) | (2\textsubscript{z} <em>0,0,0) |
| 48.2.359 | Pnnn1' | () | () | () | () | () | () |
| 48.3.360 | Pn'n'n | Pnn2 | ((0,0,0;b,c,a)) | (1</em>0,0,0) | (2\textsubscript{x} *0,0,0) | (2\textsubscript{y} *0,0,0)' | (2\textsubscript{z} <em>0,0,0)' |
| 48.4.361 | Pn'n'n | P2/c | ((1/4,1/4,1/4;b,c,a+b)) | (1</em>0,0,0) | (2\textsubscript{x} *0,0,0)' | (2\textsubscript{y} *0,0,0)' | (2\textsubscript{z} <em>0,0,0) |
| 48.5.362 | Pn'n'n | P222 | ((0,0,0;a,b,c)) | (1</em>0,0,0) | (2\textsubscript{x} *0,0,0)' | (2\textsubscript{y} *0,0,0)' | (2\textsubscript{z} <em>0,0,0) |
| 48.6.363 | P\textsubscript{F} nnn | Fddd | ((0,0,0;2a,2b,2c)) | (1</em>0,0,0) | (2\textsubscript{x} *0,0,0) | (2\textsubscript{y} *0,0,0) | (2\textsubscript{z} <em>0,0,0) |
| 49.1.364 | Pccm | () | () | (1</em>0,0,0) | (2\textsubscript{x} *0,0,1/2) | (2\textsubscript{y} *0,0,1/2) | (2\textsubscript{z} *0,0,0) |</p>
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<td>Pma2 (0,0,1/4;c,a,&amp;a)</td>
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<td>(&amp;<em>0,0,0)' (m</em>x<em>0,0,1/2)' (m</em>y<em>0,0,1/2)' (m</em>z*0,0,0)'</td>
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<td>Pc'c'm</td>
<td>P2/m (0,0,0;b,c,a)</td>
<td>(1<em>0,0,0) (2</em>x<em>0,0,1/2) (2</em>y<em>0,0,1/2) (2</em>z*0,0,0)</td>
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<td>Pc'cm'</td>
<td>P2/c (0,0,0;a,b,c)</td>
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<td>49.6.369</td>
<td>Pc'c'm'</td>
<td>P222 (0,0,0;2a,b,c)</td>
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<td>49.8.371</td>
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<td>Pccm (0,0,0;2a,b,c)</td>
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<td>Pcca (1/2,0,0;2a,b,c)</td>
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<td>P2a c'c'm</td>
<td>Pmna (0,0,0;c,b,2a)</td>
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<td>P2a c'c'm'</td>
<td>Pban (0,0,0;1/4;c,b,2a)</td>
<td>(1<em>0,0,0) (2</em>x<em>0,0,1/2) (2</em>y<em>0,0,1/2) (2</em>z*0,0,0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(&amp;<em>1,0,0)' (m</em>x<em>1,0,1/2)' (m</em>y<em>1,0,1/2)' (m</em>z*1,0,0)'</td>
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<tr>
<td>50.13.376</td>
<td>P2a ccm'</td>
<td>Ccca (1/2,1/2,1/4;2a,2b,c)</td>
<td>(1<em>0,0,0) (2</em>x<em>1,0,1/2) (2</em>y<em>1,0,1/2) (2</em>z*0,0,0)</td>
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<td>(&amp;<em>1,0,0)' (m</em>x<em>0,0,1/2)' (m</em>y<em>0,0,1/2)' (m</em>z*1,0,0)</td>
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<td>(&amp;*1/2,1/2,0)</td>
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<td>50.2.378</td>
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<td>50.3.379</td>
<td>Pb'an</td>
<td>(0,0,0;c,&amp;x,a)</td>
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<td>Pnc2</td>
<td>(1*0,0,0)</td>
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<td>50.4.380</td>
<td>Pban'</td>
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<td>Pba2</td>
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<td>P2/c</td>
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<td>(&amp;*1/2,1/2,0)'</td>
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<td>Space Group</td>
<td>Description</td>
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<td>Pmc2₁</td>
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<td>Cmcm</td>
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<td>Pbcm</td>
<td>(0,1/2,0; c,a,2b)</td>
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<td>Pmnm</td>
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<td>51.15.401</td>
<td>P&lt;sub&gt;2&lt;/sub&gt;b m'ma'</td>
<td>Pnna</td>
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<td>51.16.402</td>
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<td>Pbam</td>
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<td>Cmca</td>
<td>(0,0,1/2; 2b,2c,a)</td>
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</table>

### 52.1.406 Pnna

| 52.1.406 | Pnna | (1*0,0,0) | (2<sub>x</sub>*0,1/2,1/2) | (2<sub>y</sub>*1/2,1/2,1/2) | (2<sub>z</sub>*1/2,0,0) |
| 52.2.407 | Pnna1' |

### 52.3.408 Pn'na

| 52.3.408 | Pnc2 | (0,1/4,1/4; b,c,a) | (1*0,0,0) | (2<sub>x</sub>*0,1/2,1/2) | (2<sub>y</sub>*0,1/2,1/2) | (2<sub>z</sub>*1/2,0,0) |

### 52.4.409 Pnn'a

| 52.4.409 | Pnc2<sub>1</sub> | (1/4,0,1/4; a, b, b) | (1*0,0,0) | (2<sub>x</sub>*0,1/2,1/2) | (2<sub>y</sub>*0,1/2,1/2) | (2<sub>z</sub>*1/2,0,0) |
52.5.410  Pnna'  Pnn2  (1/4,0,0; a,b,c)  (1*0,0,0)  (2*0,1/2,1/2)  (2*1/2,1/2,1/2)  (2*1/2,0,0)  
    (&*0,0,0)' (m*0,1/2,1/2) (m*1/2,1/2,1/2) (m*1/2,0,0)'

52.6.411  Pnn'a  P2/c  (0,0,0; b,c,a)  (1*0,0,0)  (2*0,1/2,1/2)  (2*1/2,1/2,1/2)  (2*1/2,0,0)  
    (&*0,0,0)' (m*0,1/2,1/2) (m*1/2,1/2,1/2) (m*1/2,0,0)'

52.7.412  Pnn'a'  P2/c  (0,0,0; a,c,a)  (1*0,0,0)  (2*0,1/2,1/2)  (2*1/2,1/2,1/2)  (2*1/2,0,0)  
    (&*0,0,0)' (m*0,1/2,1/2) (m*1/2,1/2,1/2) (m*1/2,0,0)'

52.8.413  Pn'na'  P2/c  (1/4,0,1/4; a,b,c)  (1*0,0,0)  (2*0,1/2,1/2)  (2*1/2,1/2,1/2)  (2*1/2,0,0)  
    (&*0,0,0)' (m*0,1/2,1/2) (m*1/2,1/2,1/2) (m*1/2,0,0)'

53.1.415  Pmna  (1*0,0,0)  (2*0,0,0)  (2*1/2,0,1/2)  (2*1/2,0,1/2)  
    (&*0,0,0)' (m*0,0,0) (m*1/2,0,1/2) (m*1/2,0,1/2)'

53.2.416  Pmna1'  

53.3.417  Pmn'a  Pnc2  (0,0,0; b,c,a)  (1*0,0,0)  (2*0,0,0)  (2*1/2,0,1/2)  (2*1/2,0,1/2)  
    (&*0,0,0)' (m*0,0,0)' (m*1/2,0,1/2) (m*1/2,0,1/2)'

53.4.418  Pmna'  Pma2  (1/4,0,1/4; a,c,b)  (1*0,0,0)  (2*0,0,0)  (2*1/2,0,1/2)  (2*1/2,0,1/2)  
    (&*0,0,0)' (m*0,0,0)' (m*1/2,0,1/2) (m*1/2,0,1/2)'

53.5.419  Pmna  Pmn21  (0,0,0; a,b,c)  (1*0,0,0)  (2*0,0,0)  (2*1/2,0,1/2)  (2*1/2,0,1/2)  
    (&*0,0,0)' (m*0,0,0)' (m*1/2,0,1/2) (m*1/2,0,1/2)'

53.6.420  Pmn'a  P21/c  (0,0,0; b,c,a)  (1*0,0,0)  (2*0,0,0)  (2*1/2,0,1/2)  (2*1/2,0,1/2)  
    (&*0,0,0)' (m*0,0,0)' (m*1/2,0,1/2) (m*1/2,0,1/2)'

53.7.421  Pmn'a'  P2/m  (0,0,0; a,b,c)  (1*0,0,0)  (2*0,0,0)  (2*1/2,0,1/2)  (2*1/2,0,1/2)  
    (m*0,0,0)' (m*1/2,0,1/2) (m*1/2,0,1/2)
<p>| 53.8.422 | Pm'na' | P2/c | (0.0,0;0,0,0) | (1<em>0,0,0) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 53.9.423 | Pm'n'a' | P222 | (1/4,0,0;0,0,0) | (1<em>0,0,0) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 53.10.424 | Pm'na | Pmna | (0,0,0;0,0,0) | (1<em>0,0,0) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 53.11.425 | Pm'na | Pmna | (0,0,0;0,0,0) | (1<em>0,0,0) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 53.12.426 | Pm'na | Pmna | (0,0,0;0,0,0) | (1<em>0,0,0) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 54.1.428 | Pcca | Pcca | (1<em>0,0,0) | (2_x</em>1/2,0,1/2) | (m_x<em>0,0,0) | (m_y</em>1/2,0,1/2) | (m_z<em>1/2,0,1/2) |
| 54.2.429 | Pcca | Pcca | (1</em>0,0,0) | (2_x<em>1/2,0,1/2) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 54.3.430 | Pcc'a | Pca2 | (0,0,0;0,0,0) | (1<em>0,0,0) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 54.4.431 | Pcc'a | Pba2 | (0,0,0;0,0,0) | (1<em>0,0,0) | (m_x</em>0,0,0) | (m_y<em>1/2,0,1/2) | (m_z</em>1/2,0,1/2) |
| 54.5.432 | Pcc'a | Pcc2 | (1/4,0,0;0,0,0) | (1<em>0,0,0) | (2_x</em>1/2,0,1/2) | (m_x<em>0,0,0) | (m_y</em>1/2,0,1/2) | (m_z*1/2,0,1/2) |</p>
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<th>Basis Vectors</th>
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<td>P222_1</td>
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<th>Volume</th>
<th>Symbol</th>
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<td>Cm'ca'</td>
<td>C2/c</td>
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<td>C222 1</td>
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<td>Cp mca</td>
<td>Pbam</td>
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<td>Pnma</td>
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<td>C2/m</td>
<td>(0,0,0;b,ξ,c)</td>
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<td>Cmm'm'</td>
<td>C222</td>
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<td>Cmmm</td>
<td>(0,0,0;a,b,2c)</td>
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<td>C_p mmm</td>
<td>Pmmm</td>
<td>(0,0,0;a,b,c)</td>
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<td>Immm</td>
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<td>$(2_x*0,0,0)$</td>
<td>$(2_y*0,0,0)$</td>
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<td>$C_{2c}$ m'm'm</td>
<td>Cccm</td>
<td>$(0,0,0;a,b,2c)$</td>
<td>$(1*0,0,0)$</td>
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<td>Cmcm</td>
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<td>$C_{p}$ mm'm'</td>
<td>Pmmn</td>
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<td>$(2_y*1/2,1/2,0)$</td>
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<td>65.15.559</td>
<td>$C_{p}$ m'm'm</td>
<td>Pbam</td>
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<td>Pmna</td>
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<td>Pbam</td>
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<td>65.18.562</td>
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<td>Imma</td>
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<td>$(2_x*0,0,0)$</td>
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<td>Ibam</td>
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<td>$(2_x*0,0,1/2)$</td>
<td>$(2_y*0,0,1/2)$</td>
<td>$(2_z*0,0,0)$</td>
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</table>

66.1.564 | Cccm | $(1*0,0,0)$ | $(2_x*0,0,1/2)$ | $(2_y*0,0,1/2)$ | $(2_z*0,0,0)$ | $(m_x*0,0,1/2)$ | $(m_y*0,0,1/2)$ | $(m_z*0,0,0)$ |

66.2.565 | Cccm1’ |
66.3.566  Cc'cm  Ama2  (0,0,1/4;c,6,a)  
(1*0,0,0)  (2x*0,0,1/2)  (2y*0,0,1/2)  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.4.567  Cccm'  Ccc2  (0,0,0;a,b,c)  
(1*0,0,0)  (2x*0,0,1/2)'  (2y*0,0,1/2)'  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.5.568  Cc'c'm  P2/m  (0,0,0;b,c, {a+b}/2)  
(1*0,0,0)  (2x*0,0,1/2)'  (2y*0,0,1/2)'  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.6.569  Ccc'm'  C2/c  (0,0,0;b,a&c)  
(1*0,0,0)  (2x*0,0,1/2)'  (2y*0,0,1/2)'  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.7.570  Cc'c'm'  C222  (0,0,1/4;a,b,c)  
(1*0,0,0)  (2x*0,0,1/2)'  (2y*0,0,1/2)'  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.8.571  C_p ccm  Pccm  (0,0,0;a,b,c)  
(1*0,0,0)  (2x*0,0,1/2)  (2y*0,0,1/2)  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.9.572  C_p c'cm  Pmna  (1/4,1/4,0;c,a,b)  
(1*0,0,0)  (2x*0,0,1/2)  (2y*1/2,1/2,1/2)  (2z*1/2,1/2,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.10.573  C_p ccm'  Pccn  (1/4,1/4,0;a,b,c)  
(1*0,0,0)  (2x*1/2,1/2,1/2)  (2y*1/2,1/2,1/2)  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.11.574  C_p c'c'm  Pnnm  (0,0,0;a,b,c)  
(1*0,0,0)  (2x*1/2,1/2,1/2)  (2y*1/2,1/2,1/2)  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*0,0,1/2)'  (m*z*0,0,0)

66.12.575  C_p cc'm'  Pnna  (0,0,0;c,6,a)  
(1*0,0,0)  (2x*0,0,1/2)  (2y*1/2,1/2,1/2)  (2z*1/2,1/2,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*1/2,1/2,1/2)'  (m*z*1/2,1/2,0)

66.13.576  C_p c'c'm'  Pnnn  (0,0,1/4;a,b,c)  
(1*0,0,0)  (2x*0,0,1/2)  (2y*0,0,1/2)  (2z*0,0,0)
(6*0,0,0)'  (m*0,0,1/2)'  (m*y*1/2,1/2,1/2)'  (m*z*1/2,1/2,0)
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<p>| 72.1.630 | Ibam | (1<em>0,0,0) | (2x</em>0,0,1/2) | (2<em>0,0,1/2) | (2z</em>0,0,0) |
| 72.2.631 | Ibam1' | (m<em>0,0,1/2) | (m</em>0,0,1/2) | (m<em>0,0,0) |
| 72.3.632 | Ib'am | Ima2 | (0,0,1/4;c,Δx,a) | (1</em>0,0,0) | (2x<em>0,0,1/2) | (2</em>0,0,0) | (2z<em>0,0,0) | (m</em>0,0,1/2) | (m<em>0,0,1/2) | (m</em>0,0,0) |
| 72.4.633 | Ib'am' | Iba2 | (0,0,0;a,b,c) | (1<em>0,0,0) | (2x</em>0,0,1/2) | (2<em>0,0,0) | (2z</em>0,0,0) | (m<em>0,0,1/2) | (m</em>0,0,1/2) | (m<em>0,0,0) |
| 72.5.634 | Ib'a'm | C2/m | (0,0,0;a+b,c,a) | (1</em>0,0,0) | (2x<em>0,0,1/2) | (2</em>0,0,0) | (2z<em>0,0,0) | (m</em>0,0,1/2) | (m<em>0,0,1/2) | (m</em>0,0,0) |</p>
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<td>(1&lt;sup&gt;*&lt;/sup&gt;0,0,0)</td>
<td>(4&lt;sup&gt;*&lt;/sup&gt;0,0,1/2)</td>
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<td>P&amp;&lt;sub&gt;4&lt;/sub&gt;</td>
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<td>(m&lt;sup&gt;*&lt;/sup&gt;1/2,1/2,0)</td>
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<td>86.6.732 P4_2/n' I4_1/a</td>
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<td>(1<em>0,0,0) (4</em>1/2,1/2,1/2) (2<em>z</em>0,0,0) (4*1/2,1/2,1/2)</td>
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MAGNETIC SPACE GROUP ELEMENTS 56
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<td>P4/m</td>
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<td>91.6.769</td>
<td>P_2c, 4,22</td>
<td>6</td>
<td>(1*0, 0, 0) (2x, 0, 1/2) (2y, 0, 0)</td>
</tr>
</tbody>
</table>

MAGNETIC SPACE GROUP ELEMENTS 59
MAGNETIC SPACE GROUP ELEMENTS 60

91.7.770 P 4 \('22'\) P 4,2,2 (0,0,0;\(a-b, a+b, c\))

\[
\begin{array}{cccc}
(2x,0,0,1/2) & (2y,0,0,0) & (2xy,0,0,3/4) & (2\delta y,0,0,1/4) \\
1*0,0,0 & (4z,1/2,1/2,1/4) & (2,0,0,1/2) & (4z,1*1/2,1/2,3/4) \\
2x,0,0,1/2 & (2y,0,0,0) & (2xy,1/2,3/4) & (2\delta y,0,0,1/2) \\
\end{array}
\]

92.1.771 P 4,2,2

\[
\begin{array}{cccc}
(1*0,0,0) & (4z,1/2,1/2,1/4) & (2,0,0,1/2) & (4z,1*1/2,1/2,3/4) \\
2x,1/2,1/2,3/4 & (2y,1/2,1/2,1/4) & (2xy,0,0,0) & (2\delta y,0,0,1/2) \\
\end{array}
\]

92.2.772 P 4,2,21'

92.3.773 P 4,1,2,2' P 2,2,2 (1/4, 0, 1/8; a, b, c)

\[
\begin{array}{cccc}
(1*0,0,0) & (4z,1/2,1/2,1/4)' & (2,0,0,1/2) & (4z,1*1/2,1/2,3/4)' \\
2x,1/2,1/2,3/4 & (2y,1/2,1/2,1/4)' & (2xy,0,0,0)' & (2\delta y,0,0,1/2)' \\
\end{array}
\]

92.4.774 P 4,1,2,2' P 4,1 (1/2, 0, 0; a, b, c)

\[
\begin{array}{cccc}
(1*0,0,0) & (4z,1/2,1/2,1/4)' & (2,0,0,1/2) & (4z,1*1/2,1/2,3/4)' \\
2x,1/2,1/2,3/4' & (2y,1/2,1/2,1/4)' & (2xy,0,0,0)' & (2\delta y,0,0,1/2)' \\
\end{array}
\]

92.5.775 P 4,1,2,2' C 222,1 (0, 0, 0; a+b, -a-b, c)

\[
\begin{array}{cccc}
(1*0,0,0) & (4z,1/2,1/2,1/4)' & (2,0,0,1/2) & (4z,1*1/2,1/2,3/4)' \\
2x,1/2,1/2,3/4' & (2y,1/2,1/2,1/4)' & (2xy,0,0,0)' & (2\delta y,0,0,1/2)' \\
\end{array}
\]

93.1.776 P 4,2,2

\[
\begin{array}{cccc}
(1*0,0,0) & (4z,0,0,1/2) & (2,0,0,0) & (4z,1*0,0,1/2) \\
2x,0,0,0 & (2y,0,0,0) & (2xy,0,0,1/2) & (2\delta y,0,0,1/2) \\
\end{array}
\]

93.2.777 P 4,2,21'

93.3.778 P 4,2,2' P 222 (0, 0, 0; a, b, c)

\[
\begin{array}{cccc}
(1*0,0,0) & (4z,0,0,1/2)' & (2,0,0,0) & (4z,1*0,0,1/2)' \\
2x,0,0,0 & (2y,0,0,0) & (2xy,0,0,1/2)' & (2\delta y,0,0,1/2)' \\
\end{array}
\]

93.4.779 P 4,2,2' P 4,2 (0, 0, 0; a, b, c)

\[
\begin{array}{cccc}
(1*0,0,0) & (4z,0,0,1/2)' & (2,0,0,0) & (4z,1*0,0,1/2)' \\
2x,0,0,0' & (2y,0,0,0)' & (2xy,0,0,1/2)' & (2\delta y,0,0,1/2)' \\
\end{array}
\]
<table>
<thead>
<tr>
<th>Code</th>
<th>Space Group</th>
<th>Elements</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>93.5.780</td>
<td>P4₂2'2</td>
<td>C222</td>
<td>(0,0,1/4; a-b, a+b, c)</td>
</tr>
<tr>
<td>93.6.781</td>
<td>P₃c 4₂ 22</td>
<td>P4₂2</td>
<td>(0,0,0; b, a, c)</td>
</tr>
<tr>
<td>93.7.782</td>
<td>P₃ 4₂ 22</td>
<td>P4₂2</td>
<td>(0,0,1/4; a-b, a+b, c)</td>
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<tr>
<td>93.8.783</td>
<td>P₈ 4₂ 22</td>
<td>I4₂2</td>
<td>(-1/2,0,0; a-b, a+b, c)</td>
</tr>
<tr>
<td>93.9.784</td>
<td>P₃c 4₂'22'</td>
<td>P₄₃ 22</td>
<td>(0,0,0; b, a, c)</td>
</tr>
<tr>
<td>94.1.786</td>
<td>P4₂ 2,2</td>
<td>(1*0,0,0)</td>
<td>(4_z*0,1/2)</td>
</tr>
<tr>
<td>94.2.787</td>
<td>P4₂ 2,2'1'</td>
<td>(2*0,1/2,1/2,1/2)</td>
<td>(2*0,0,0)</td>
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<tr>
<td>94.3.788</td>
<td>P₄₂ 2,2'</td>
<td>P₂₁₂₂</td>
<td>(0,0,1/4; a, b, c)</td>
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<tr>
<td>94.4.789</td>
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<td>P₄₂</td>
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</tr>
<tr>
<td>94.5.790</td>
<td>P₄₂ 2,2'</td>
<td>C222</td>
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</tr>
<tr>
<td>94.6.791</td>
<td>P₂₃ 4₂ 2,2</td>
<td>P₄₂ 2,2</td>
<td>(0,0,0; b, a, c)</td>
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MAGNETIC SPACE GROUP ELEMENTS 61
<table>
<thead>
<tr>
<th>Magnetic Space Group Elements</th>
<th>Pnma 2</th>
<th>P43 2</th>
<th>(0,0,0;b,c)</th>
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<tr>
<td>95.792</td>
<td>P2c 4</td>
<td>P43 2</td>
<td>(0,0,0;b,c)</td>
</tr>
<tr>
<td>95.1793</td>
<td>P43 22</td>
<td>(1*0,0,0)</td>
<td>(2*0,1/2,1/2)</td>
</tr>
<tr>
<td>95.2.794</td>
<td>P43 221</td>
<td>(0,0,0;b,c)</td>
<td></td>
</tr>
<tr>
<td>95.3.795</td>
<td>P43'22'</td>
<td>(0,0,0;b,c)</td>
<td></td>
</tr>
<tr>
<td>95.4.796</td>
<td>P43 2'2'</td>
<td>(0,0,0;a,b,c)</td>
<td></td>
</tr>
<tr>
<td>95.5.797</td>
<td>P43 2'2</td>
<td>(0,0,0;a-b,a+b,c)</td>
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</tr>
<tr>
<td>95.6.798</td>
<td>P43 22</td>
<td>(0,0,0;a+b,-a+b,c)</td>
<td></td>
</tr>
<tr>
<td>95.7.799</td>
<td>P43'22'</td>
<td>(0,0,0;a+b,-a+b,c)</td>
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</tr>
<tr>
<td>96.1.800</td>
<td>P43 2</td>
<td>(1*0,0,0)</td>
<td>(2*1/2,1/2,1/2)</td>
</tr>
<tr>
<td>96.2.801</td>
<td>P43 21</td>
<td>(0,0,0;1/2,1/2,1/2)</td>
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</tr>
<tr>
<td>96.3.802</td>
<td>P4₃'2,2'</td>
<td>P2,2,2₁</td>
<td>(1/4,0,-1/8;a,b,c)</td>
</tr>
<tr>
<td>96.4.803</td>
<td>P4₃ 2₁'2'</td>
<td>P4₃</td>
<td>(1/2,0,0;a,b,c)</td>
</tr>
<tr>
<td>96.5.804</td>
<td>P4₃ 2₁'2'</td>
<td>C222₁</td>
<td>(0,0,0;a+b,-a+b,c)</td>
</tr>
<tr>
<td>97.1.805</td>
<td>I422</td>
<td>(1⁺₀,₀,₀)</td>
<td>(4₂⁻¹⁺₁/₂,1/₂,3/₄)</td>
</tr>
<tr>
<td>97.2.806</td>
<td>I422₁'</td>
<td>(1⁺₀,₀,₀)</td>
<td>(4₂⁻¹⁺₁/₂,1/₂,3/₄)</td>
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<tr>
<td>97.3.807</td>
<td>I4'22'</td>
<td>I222</td>
<td>(0,0,0;a,b,c)</td>
</tr>
<tr>
<td>97.4.808</td>
<td>I42'2'</td>
<td>I4</td>
<td>(0,0,0;a,b,c)</td>
</tr>
<tr>
<td>97.5.809</td>
<td>I4'2'2'</td>
<td>F222</td>
<td>(0,0,0;a-b,a+b,c)</td>
</tr>
<tr>
<td>97.6.810</td>
<td>Iₚ 422</td>
<td>P422</td>
<td>(0,0,0;a,b,c)</td>
</tr>
<tr>
<td>97.7.811</td>
<td>Iₚ 4'22'</td>
<td>P4₂22</td>
<td>(1/2,0,0;a,b,c)</td>
</tr>
<tr>
<td>97.8.812</td>
<td>Iₚ 42'2'</td>
<td>P4₂,2</td>
<td>(1/2,0,1/₄;a,b,c)</td>
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<tr>
<td>97.9.813</td>
<td>I_p 4'2'2</td>
<td>P4_212</td>
<td>(0,0,0;a,b,c)</td>
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<tr>
<td>98.1.814</td>
<td>I4,22</td>
<td>(1*0,0,0)</td>
<td>(4_z*0,1/2,1/4)</td>
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<tr>
<td>98.2.815</td>
<td>I4,221'</td>
<td>(1*0,0,0)</td>
<td>(4_z*0,1/2,1/4)</td>
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<td>98.3.816</td>
<td>I4,'22'</td>
<td>I2,2,2_1</td>
<td>(0,1/4,1/4;a,b,c)</td>
</tr>
<tr>
<td>98.4.817</td>
<td>I4,2'2'</td>
<td>I4,1</td>
<td>(1/4,-1/4,0;a,b,c)</td>
</tr>
<tr>
<td>98.5.818</td>
<td>I4,'2'2'</td>
<td>F222</td>
<td>(0,0,0;a-b,a+b,c)</td>
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<tr>
<td>98.6.819</td>
<td>I_p 4,22</td>
<td>P4,22</td>
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<tr>
<td>98.7.820</td>
<td>I_p 4,'22'</td>
<td>P4_3 22</td>
<td>(1/4,1/4,1/8;a,b,c)</td>
</tr>
<tr>
<td>98.8.821</td>
<td>I_p 4,2'2'</td>
<td>P4,2,2</td>
<td>(1/4,1/4,0;a,b,c)</td>
</tr>
<tr>
<td>98.9.822</td>
<td>I_p 4,'2'2'</td>
<td>P4_3 2,2</td>
<td>(1/4,-1/4,1/4;a,b,c)</td>
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<tr>
<td>99.1.823</td>
<td>P4mm</td>
<td>(1*0,0,0)</td>
<td>(4_z*0,0,0)</td>
</tr>
<tr>
<td>Number</td>
<td>Symbol</td>
<td>Point Group</td>
<td>Basis Vectors</td>
</tr>
<tr>
<td>-------</td>
<td>---------</td>
<td>-------------</td>
<td>---------------</td>
</tr>
</tbody>
</table>
| 99.2.824 | P4mm1' | Cmm2 | (0,0,0; a-b, a+b, c) | (1\*0,0,0) (4\_z\*0,0,0)' (2\*0,0,0) (4\_z\^1\*0,0,0)'
|          |         |             |               | (m\_x\*0,0,0)' (m\_y\*0,0,0)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0)'
| 99.3.825 | P4'm'm Cmm2 | (0,0,0; a, b, c) | (1\*0,0,0) (4\_z\*0,0,0)' (2\*0,0,0) (4\_z\^1\*0,0,0)'
|          |         |             |               | (m\_x\*0,0,0)' (m\_y\*0,0,0)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0)'
| 99.4.826 | P4'm'm' Pmm2 | (0,0,0; a-b, a+b, c) | (1\*0,0,0) (4\_z\*0,0,0)' (2\*0,0,0) (4\_z\^1\*0,0,0)'
|          |         |             |               | (m\_x\*0,0,0)' (m\_y\*0,0,0)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0)'
| 99.5.827 | P4m'm' P4 | (0,0,0; a-b, a+b, c) | (1\*0,0,0) (4\_z\*0,0,0)' (2\*0,0,0) (4\_z\^1\*0,0,0)'
|          |         |             |               | (m\_x\*0,0,0)' (m\_y\*0,0,0)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0)'
| 99.6.828 | P2c 4mm P4mm | (0,0,0; a, b, 2c) | (1\*0,0,0) (4\_z\*0,0,0)' (2\*0,0,0) (4\_z\^1\*0,0,0)'
|          |         |             |               | (m\_x\*0,0,0)' (m\_y\*0,0,0)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0)'
| 99.7.829 | P\_p4mm P4mm | (0,0,0; a-b, a+b, c) | (1\*0,0,0) (4\_z\*0,0,0)' (2\*0,0,0) (4\_z\^1\*0,0,0)'
|          |         |             |               | (m\_x\*0,0,0)' (m\_y\*0,0,0)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0)'
| 99.8.830 | P\_14mm I4mm | (0,0,0; a-b, a+b, 2c) | (1\*0,0,0) (4\_z\*0,0,0)' (2\*0,0,0) (4\_z\^1\*0,0,0)'
|          |         |             |               | (m\_x\*0,0,0)' (m\_y\*0,0,0)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0)'
| 99.9.831 | P2c 4'm'm P4\_2cm | (0,0,0; a, b, 2c) | (1\*0,0,0) (4\_z\*0,0,0,01) (2\*0,0,0) (4\_z\^1\*0,0,01)
|          |         |             |               | (m\_x\*0,0,0,1)' (m\_y\*0,0,0,1)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0,1)'
| 99.10.832 | P2c 4'm'm' P4\_2mc | (0,0,0; a, b, 2c) | (1\*0,0,0) (4\_z\*0,0,0,01) (2\*0,0,0) (4\_z\^1\*0,0,01)
|          |         |             |               | (m\_x\*0,0,0,1)' (m\_y\*0,0,0,1)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0,1)'
| 99.11.833 | P2c 4'm'm' P4cc | (0,0,0; a, b, 2c) | (1\*0,0,0) (4\_z\*0,0,0,0) (2\*0,0,0) (4\_z\^1\*0,0,0,0)
|          |         |             |               | (m\_x\*0,0,0,1)' (m\_y\*0,0,0,1)' (m\_z\*0,0,0) (m\_x\^1\*0,0,0,1)'
| 99.12.834 | P\_p4'm'm' P4bm | (1/2, 1/2, 0; a-b, a+b, c) | (1\*0,0,0) (4\_z\*1,0,0) (2\*0,0,0) (4\_z\^1\*1,0,0)
|          |         |             |               | (m\_x\*0,0,0) (m\_y\*0,0,0) (m\_z\*1,0,0) (m\_x\^1\*1,0,0)'
| 99.13.835 | P\_14'm'm' I4cm | (0,0,0; a-b, a+b, 2c) | (1\*0,0,0) (4\_z\*0,0,0) (2\*0,0,0) (4\_z\^1\*0,0,0)
|          |         |             |               | (m\_x\*1,0,0) (m\_y\*1,0,0) (m\_z\*1,0,0) (m\_x\^1,0,0)'

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<table>
<thead>
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<th>100.1.836</th>
<th>P4bm</th>
<th>((1*0,0,0))</th>
<th>((4_z*0,0,0))</th>
<th>((2_z*0,0,0))</th>
<th>((4_z^{-1}*0,0,0))</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>((m_x*1/2,1/2,0))</td>
<td>((m_y*1/2,1/2,0))</td>
<td>((m_{xy}*1/2,1/2,0))</td>
<td>((m_{sy}*1/2,1/2,0))</td>
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<td>((4_z*0,0,0))</td>
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<td>((4_z^{-1}*0,0,0))</td>
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<td>((m_x*1/2,1/2,0)')</td>
<td>((m_y*1/2,1/2,0)')</td>
<td>((m_{xy}*1/2,1/2,0)')</td>
<td>((m_{sy}*1/2,1/2,0)')</td>
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<td>100.3.838</td>
<td>P4'b'm</td>
<td>Cmm2</td>
<td>((1/2,0,0;a-b,a+b,c))</td>
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<td>((4_z*0,0,0))</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((m_x*1/2,1/2,0)')</td>
<td>((m_y*1/2,1/2,0)')</td>
<td>((m_{xy}*1/2,1/2,0)')</td>
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<td>Pba2</td>
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<td>((4_z*0,0,0))</td>
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<tr>
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<td></td>
<td>((m_x*1/2,1/2,0)')</td>
<td>((m_y*1/2,1/2,0)')</td>
<td>((m_{xy}*1/2,1/2,0)')</td>
<td>((m_{sy}*1/2,1/2,0)')</td>
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<td>100.5.840</td>
<td>P4b'm'</td>
<td>P4</td>
<td>((0,0,0;a,b,c))</td>
<td>((1*0,0,0))</td>
<td>((4_z*0,0,0))</td>
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<td>((m_x*1/2,1/2,0)')</td>
<td>((m_y*1/2,1/2,0)')</td>
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<td>P4bm</td>
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<td>((m_y*1/2,1/2,0)')</td>
<td>((m_{xy}*1/2,1/2,0)')</td>
<td>((m_{sy}*1/2,1/2,0)')</td>
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<td>P4₂nm</td>
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<td>((4_z*0,0,0))</td>
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<tr>
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<td>((m_x*1/2,1/2,1))</td>
<td>((m_y*1/2,1/2,1))</td>
<td>((m_{xy}*1/2,1/2,0))</td>
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<td>100.8.843</td>
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<td>P4₂bc</td>
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<td>((4_z*0,0,0))</td>
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<tr>
<td></td>
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<td>((m_x*1/2,1/2,0)')</td>
<td>((m_y*1/2,1/2,0)')</td>
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<td>((4_z^{-1}*0,0,0))</td>
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<td>((m_y*0,0,1/2))</td>
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<td>P4₂ cm1'</td>
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<td>Ccc²</td>
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<td>(4⁻¹*0,0,0)</td>
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MAGNETIC SPACE GROUP ELEMENTS 68
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<td>(4z*0,0,0)</td>
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<td>(mᵧ*1/2,1/2,1/2)</td>
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<td>I4cm1'</td>
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<td>I4'c'm</td>
<td>Fmm2</td>
<td>(1/2,0,0;a-b,a+b,c) (1<em>0,0,0) (4z</em>0,0,0) (m_x *1/2,1/2,0) (m_y <em>1/2,1/2,0) (2</em>0,0,0) (m_xy <em>1/2,1/2,0) (4z-1</em>0,0,0) (m_xy *1/2,1/2,0)</td>
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<td>Iba2</td>
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<td>I4</td>
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<td>P4_2cm</td>
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<td>P4cc</td>
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<td>Fdd2</td>
<td>(0,0,0;a-b,a+b,c) (1<em>0,0,0) (4z</em>0,0,0) (m_x *0,0,0) (m_y <em>0,0,0) (2</em>0,0,0) (m_xy <em>0,0,0) (4z-1</em>0,0,0) (m_xy *0,0,0)</td>
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MAGNETIC SPACE GROUP ELEMENTS 71
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| 109.5.905 | I4,m'd' | I4 | (1/4,-1/4,0; a,b,c) | (1<em>0,0,0) | (4_z</em>0,1/2,1/4)' | (2_z<em>0,0,0) | (4_z-1</em>0,1/2,1/4)' | (m_x<em>0,0,0) | (m_y</em>0,0,0) | (m_x<em>0,1/2,1/4)' | (m_y</em>0,1/2,1/4) |
| 110.1.906 | I4,cd |  |  | (1<em>0,0,0) | (4_z</em>0,1/2,1/4)' | (2_z<em>0,0,0) | (4_z-1</em>0,1/2,1/4)' | (m_x<em>0,0,1/2) | (m_y</em>0,0,1/2) | (m_x<em>0,1/2,3/4) | (m_y</em>0,1/2,3/4) |
| 110.2.907 | I4,cd1' |  |  |  |  |  |  |  |  |  |  |
| 110.3.908 | I4,'c'd | Fdd2 | (0,0,0; a-b,a+b,c) | (1<em>0,0,0) | (4_z</em>0,1/2,1/4)' | (2_z<em>0,0,0) | (4_z-1</em>0,1/2,1/4)' | (2x<em>0,0,0) | (2y</em>0,0,0) | (m_xy<em>0,0,0) | (m_x</em>0,0,0) |
| 110.4.909 | I4,'cd' | Iba2 | (0,0,0; a,b,c) | (1<em>0,0,0) | (4_z</em>0,1/2,1/4)' | (2_z<em>0,0,0) | (4_z-1</em>0,1/2,1/4)' | (m_x<em>0,0,1/2) | (m_y</em>0,0,1/2) | (m_x<em>0,1/2,3/4) | (m_y</em>0,1/2,3/4) |
| 110.5.910 | I4,'c'd' | I4 | (1/4,-1/4,0; a,b,c) | (1<em>0,0,0) | (4_z</em>0,1/2,1/4)' | (2_z<em>0,0,0) | (4_z-1</em>0,1/2,1/4)' | (m_x<em>0,0,1/2) | (m_y</em>0,0,1/2) | (m_x<em>0,1/2,3/4) | (m_y</em>0,1/2,3/4) |
| 111.1.911 | P&amp;2m |  |  | (1<em>0,0,0) | (4_z</em>0,0,0) | (2_z<em>0,0,0) | (4_z-1</em>0,0,0) | (2x<em>0,0,0) | (2y</em>0,0,0) | (m_xy<em>0,0,0) | (m_y</em>0,0,0) |
| 111.2.912 | P&amp;2m1' |  |  |  |  |  |  |  |  |  |  |
| 111.3.913 | P&amp;2'm | Cmm2 | (0,0,0; a-b,a+b,c) | (1<em>0,0,0) | (4_z</em>0,0,0)' | (2_z<em>0,0,0) | (4_z-1</em>0,0,0)' | (2x<em>0,0,0)' | (2y</em>0,0,0)' | (m_xy<em>0,0,0) | (m_y</em>0,0,0) |
| 111.4.914 | P&amp;2'm' | P222 | (0,0,0; a,b,c) | (1<em>0,0,0) | (4_z</em>0,0,0)' | (2_z<em>0,0,0) | (4_z-1</em>0,0,0)' | (2x<em>0,0,0)' | (2y</em>0,0,0)' | (m_xy<em>0,0,0) | (m_y</em>0,0,0)' |</p>
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<th>Magnetism</th>
<th>Representative Translations</th>
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<td>(1*0,0,0)</td>
<td>(2_x*0,0,0)' (2_y^<em>0,0,0)' (2_z</em>0,0,0)</td>
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MAGNETIC SPACE GROUP ELEMENTS 73
112.6.927  \( \text{P\&2c} \)  \( \text{P\&c2} \)  \((0,0,0; a-b, a+b, c)\)  
\((1^*0,0,0)\)  
\((\mathbf{g}\_z^*0,0,0)\)  
\((2^*0,0,0)\)  
\((\mathbf{g}\_z^{-1}*0,0,0)\)  
\((m\_x*0,0,1/2)\)  
\((m\_y*0,0,1/2)\)  
\((m\_z*0,0,1/2)\)  
\((2^*0,0,1/2)\)  
\((2^*0,0,1/2)\)  
\((m\_y*0,0,1/2)\)  
\((m\_z*0,0,1/2)\)

112.7.928  \( \text{P\&'2c'} \)  \( \text{P\&n2} \)  \((1/2,-1/2,0; a-b, a+b, c)\)  
\((1^*0,0,0)\)  
\((\mathbf{g}\_x^*1,0,0)\)  
\((2^*0,0,0)\)  
\((\mathbf{g}\_z^{-1}*1,0,0)\)  
\((m\_x^1,0,1/2)\)  
\((m\_y^1,0,1/2)\)  
\((m\_z^1,0,1/2)\)  
\((2^*0,0,1/2)\)  
\((2^*0,0,1/2)\)  
\((m\_y^1,0,1/2)\)  
\((m\_z^1,0,1/2)\)

113.1.929  \( \text{P\&2,m} \)  
\((1^*0,0,0)\)  
\((\mathbf{g}\_x^*0,0,0)\)  
\((2^*0,0,0)\)  
\((\mathbf{g}\_z^{-1}*0,0,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)

113.2.930  \( \text{P\&2,m1'} \)  

113.3.931  \( \text{P\&'2,m} \)  \( \text{Cmm2} \)  \((1/2,0,0; a-b, a+b, c)\)  
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\((\mathbf{g}\_x^*0,0,0)\)  
\((2^*0,0,0)\)  
\((\mathbf{g}\_z^{-1}*0,0,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)  
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\((m\_z^*1/2,1/2,0)\)

113.4.932  \( \text{P\&'2,m'} \)  \( \text{P2122} \)  \((0,0,0; a, b, c)\)  
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\((\mathbf{g}\_x^*0,0,0)\)  
\((2^*0,0,0)\)  
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\((m\_z^*1/2,1/2,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)

113.5.933  \( \text{P\&2,m'} \)  \( \text{P}\)  \((0,0,0; a, b, c)\)  
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\((\mathbf{g}\_x^*0,0,0)\)  
\((2^*0,0,0)\)  
\((\mathbf{g}\_z^{-1}*0,0,0)\)  
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\((m\_z^*1/2,1/2,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)

113.6.934  \( \text{P}_{2c} \&2,m \)  \( \text{P}\&2,m \)  \((0,0,0; a, b, 2c)\)  
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\((\mathbf{g}\_x^*0,0,0)\)  
\((2^*0,0,0)\)  
\((\mathbf{g}\_z^{-1}*0,0,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)

113.7.935  \( \text{P}_{2c} \&'2,m' \)  \( \text{P}\&2,c \)  \((0,0,1/2; a, b, 2c)\)  
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\((\mathbf{g}\_x^*0,0,0)\)  
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\((\mathbf{g}\_z^{-1}*0,0,0)\)  
\((m\_y^*1/2,1/2,0)\)  
\((m\_z^*1/2,1/2,0)\)  
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114.1.936  \( \text{P}\&2,c \)  
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118.6.970 Pm2d 0,0,0;a-b,a+b,2c

119.1.971 I\(\bar{m}\)2 (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

119.2.972 \(\bar{m}\)21' (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

119.3.973 Im2 (0,0,0; a,b,c) (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

119.4.974 \(\bar{m}\)2 (0,0,0; a,b,c) (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

119.5.975 \(\bar{m}\)2 (0,0,0; a,b,c) (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

119.6.976 \(\bar{m}\)2 (0,0,0; a,b,c) (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

119.7.977 \(\bar{m}\)2 (1/2,0,1/4; a,b,c) (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

120.1.978 \(\bar{m}\)2 (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

120.2.979 \(\bar{m}\)21' (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)

120.3.980 \(\bar{m}\)2 (0,0,1/4; a-b,a+b,c) (1,0,0,0) (m_ż,0,0,0) (2,0,0,0) (m_ż',0,0,0)
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| 130.4.1091 | P4'/nc'c | Ccca | (0,0,1/4;a-b,a+b,c) | \(
\begin{align*}
(\mathbf{A}_x^{1/2,1/2,0})' \quad (\mathbf{A}_y^{0,0,0})' \\
(m_x^{0,0,1/2}) \quad (m_y^{0,0,1/2}) \quad (m_z^{1/2,1/2,0}) \quad (\mathbf{A}_z^{1/2,1/2,0})'
\end{align*}
|}

| 130.5.1092 | P4'/ncc' | Pccn | (1/4,1/4,0;a,b,c) | \(
\begin{align*}
(1^*0,0,0) \quad (4_z^{1/2,1/2,0})' \\
(2_x^{1/2,1/2,1/2})' \quad (2_y^{1/2,1/2,1/2})' \\
(\mathbf{A}_x^{1/2,1/2,0})' \quad (\mathbf{A}_y^{0,0,0})' \\
(m_x^{0,0,1/2})' \quad (m_y^{0,0,1/2}) \quad (m_z^{1/2,1/2,0}) \quad (\mathbf{A}_z^{1/2,1/2,0})'
\end{align*}
|}

| 130.6.1093 | P4'/n'c'c | P\&2,c | (0,0,0;a,b,c) | \(
\begin{align*}
(1^*0,0,0) \quad (4_z^{1/2,1/2,0})' \\
(2_x^{1/2,1/2,1/2})' \quad (2_y^{1/2,1/2,1/2})' \\
(\mathbf{A}_x^{1/2,1/2,0})' \quad (\mathbf{A}_y^{0,0,0})' \\
(m_x^{0,0,1/2})' \quad (m_y^{0,0,1/2}) \quad (m_z^{1/2,1/2,0}) \quad (\mathbf{A}_z^{1/2,1/2,0})'
\end{align*}
|}

| 130.7.1094 | P4/nc'c' | P4/n | (0,0,0;a,b,c) | \(
\begin{align*}
(1^*0,0,0) \quad (4_z^{1/2,1/2,0})' \\
(2_x^{1/2,1/2,1/2})' \quad (2_y^{1/2,1/2,1/2})' \\
(\mathbf{A}_x^{1/2,1/2,0})' \quad (\mathbf{A}_y^{0,0,0})' \\
(m_x^{0,0,1/2})' \quad (m_y^{0,0,1/2}) \quad (m_z^{1/2,1/2,0}) \quad (\mathbf{A}_z^{1/2,1/2,0})'
\end{align*}
|}

| 130.8.1095 | P4'/n'cc' | P\&c2 | (0,0,0;a,b,c) | \(
\begin{align*}
(1^*0,0,0) \quad (4_z^{1/2,1/2,0})' \\
(2_x^{1/2,1/2,1/2})' \quad (2_y^{1/2,1/2,1/2})' \\
(\mathbf{A}_x^{1/2,1/2,0})' \quad (\mathbf{A}_y^{0,0,0})' \\
(m_x^{0,0,1/2})' \quad (m_y^{0,0,1/2}) \quad (m_z^{1/2,1/2,0}) \quad (\mathbf{A}_z^{1/2,1/2,0})'
\end{align*}
|}

| 130.9.1096 | P4/n'c'c' | P42,2 | (0,0,1/4;a,b,c) | \(
\begin{align*}
(1^*0,0,0) \quad (4_z^{1/2,1/2,0})' \\
(2_x^{1/2,1/2,1/2}) \quad (2_y^{1/2,1/2,1/2}) \quad (2_z^{0,0,0}) \quad (\mathbf{A}_z^{1/2,1/2,0})'
\end{align*}
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<td>(2*0,0,0)</td>
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<td>(2*0,0,0)</td>
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### 132.2.1111 P4₂/mcm1'

### 132.3.1112 P4₂/m'cm P4₂ cm

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### 132.5.1114 P4₂ '/mc'm Pcmm

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### 132.6.1115 P4₂ '/mc'm P42m

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### 132.7.1116 P4₂/mc'm P4₂/m

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### 132.8.1117 P4₂ '/m'c'm P4₂/c2

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<td>1/2,0,1/4; a,b,c</td>
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<td>(1*0,0,0)</td>
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<td>(2_x*0,0,1/2)</td>
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<tr>
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<td>(∂*1/2,1/2,1/2)'</td>
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<tr>
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<td>(m_x*1/2,1/2,0)'</td>
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<td>(2_y*0,0,1/2)</td>
</tr>
<tr>
<td></td>
<td>(∂*0,0,0)'</td>
</tr>
<tr>
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<td>(m_x*1/2,1/2,0)'</td>
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</table>

| P4 2/nmm             | 134.1.1132 | P4 2/nmm |
|                     | 0,0,0; a,b,c |
|                     | (1*0,0,0) | (4_z*1/2,1/2,1/2) |
|                     | (2_x*0,0,0) | (2_y*0,0,0) |
|                     | (∂*1/2,1/2,1/2) | (∂*0,0,0) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |
|                     | (2_y*0,0,0) | (2_x*0,0,0) |
|                     | (∂*0,0,0) | (∂*1/2,1/2,1/2) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |

| P4 2/n'm              | 134.2.1133 | P4 2/n'm 1 |
|                     | 0,0,0; a,b,c |
|                     | (1*0,0,0) | (4_z*1/2,1/2,1/2) |
|                     | (2_x*0,0,0) | (2_y*0,0,0) |
|                     | (∂*1/2,1/2,1/2) | (∂*0,0,0) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |
|                     | (2_y*0,0,0) | (2_x*0,0,0) |
|                     | (∂*0,0,0) | (∂*1/2,1/2,1/2) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |

| P4 2'/nn'm            | 134.4.1135 | Cmma (1/4,1/4,1/4; a-b,a+b,c) |
|                     | 1/4,1/4,1/4; a-b,a+b,c |
|                     | (1*0,0,0) | (4_z*1/2,1/2,1/2) |
|                     | (2_x*0,0,0) | (2_y*0,0,0) |
|                     | (∂*1/2,1/2,1/2) | (∂*0,0,0) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |
|                     | (2_y*0,0,0) | (2_x*0,0,0) |
|                     | (∂*0,0,0) | (∂*1/2,1/2,1/2) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |

| P4 2'/nn'm            | 134.5.1136 | Pnnn (0,0,0; a,b,c) |
|                     | 0,0,0; a,b,c |
|                     | (1*0,0,0) | (4_z*1/2,1/2,1/2) |
|                     | (2_x*0,0,0) | (2_y*0,0,0) |
|                     | (∂*1/2,1/2,1/2) | (∂*0,0,0) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |
|                     | (2_y*0,0,0) | (2_x*0,0,0) |
|                     | (∂*0,0,0) | (∂*1/2,1/2,1/2) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |

| P4 2'/n'n'm           | 134.6.1137 | P&2m (0,0,0; a,b,c) |
|                     | 0,0,0; a,b,c |
|                     | (1*0,0,0) | (4_z*1/2,1/2,1/2) |
|                     | (2_x*0,0,0) | (2_y*0,0,0) |
|                     | (∂*1/2,1/2,1/2) | (∂*0,0,0) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |
|                     | (2_y*0,0,0) | (2_x*0,0,0) |
|                     | (∂*0,0,0) | (∂*1/2,1/2,1/2) |
|                     | (m_x*1/2,1/2,1/2) | (m_y*1/2,1/2,1/2) |
| P4<sub>2</sub>/nn'm' | P4<sub>2</sub>/n | (0,0,0;a,b,c) | (1*0,0,0) | (4<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (2<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>) | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sup>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' |
| P4<sub>2</sub>'/n'm' | P4<sub>2</sub>/nn2 | (0,0,0;a,b,c) | (1*0,0,0) | (4<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (2<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>) | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sup>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' |
| P4<sub>2</sub>/n'm' | P4<sub>2</sub>/22 | (1/2,0,0;a,b,c) | (1*0,0,0) | (4<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (2<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>) | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sup>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' |
| P4<sub>1</sub>4<sub>2</sub>/nnm | I4<sub>1</sub>/amd | (0,0,0;a-b,a+b,2c) | (1*0,0,0) | (4<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (2<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>) | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sup>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' |
| P4<sub>1</sub>4<sub>2</sub>/nn'm' | I4<sub>1</sub>/acd | (0,0,0;a-b,a+b,2c) | (1*0,0,0) | (4<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (2<sub>z</sub>*</sub><sup>1/2,1/2,1/2</sup>) | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>) | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sup>)' | (2<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (4<sub>v</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sup>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>) | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>x</sub>*)<sup>1/2,1/2,1/2</sub>)' | (m<sub>y</sub>*)<sup>1/2,1/2,1/2</sub>)' |

\[135.1.1143\] P4<sub>2</sub>/mbc

\[135.2.1144\] P4<sub>2</sub>/mbc1'
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<td>135.3.1145</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/m'bc</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;bc (0,0,0; a,b,c) (1<em>0,0,0) (2</em>1/2,1/2,0) (2<em>1/2,0,0) (4</em>0,0,0) (2<em>z</em>0,0,1/2)</td>
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<td></td>
<td></td>
<td>(2<em>x</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,0)* (2<em>z</em>1/2,1/2,1/2)* (m<em>0,0,0)</em> (m<em>z</em>1/2,1/2,0)*</td>
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<td></td>
<td>(m<em>x</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,0) (m<em>z</em>1/2,1/2,1/2) (m<em>y</em>1/2,1/2,2)*</td>
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<td>135.4.1146</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/mb'c</td>
<td>Cccm (1/2,0,0; a-b,a+b,c) (1<em>0,0,0) (4</em>0,0,1/2) (2<em>z</em>0,0,0) (2<em>z</em>1/2,1/2,1/2) (m*0,0,0)</td>
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<td></td>
<td>(4<em>1,0,0,1/2) (2</em>y<em>1/2,1/2,0)</em> (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,1/2)* (m<em>z</em>0,0,0)*</td>
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<tr>
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<td>(m<em>z</em>1/2,1/2,1/2) (m<em>y</em>1/2,1/2,1/2)</td>
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<td>135.5.1147</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/m'bc</td>
<td>Pbam (0,0,0; a,b,c) (1<em>0,0,0) (2</em>z<em>0,0,1/2) (2</em>z<em>1/2,1/2,0) (2</em>y<em>0,0,0) (2</em>x*0,0,0)</td>
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<td>(2<em>x</em>1/2,1/2,2)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,1/2)*</td>
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<td>(m<em>x</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,1/2)</td>
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<td>135.6.1148</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/m'b'c</td>
<td>P&amp;2,c (0,0,1/4; a,b,c) (1<em>0,0,0) (2</em>z<em>0,0,1/2) (2</em>z<em>1/2,1/2,0) (2</em>y<em>0,0,0) (2</em>x*0,0,0)</td>
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<td>(2<em>x</em>1/2,1/2,2)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,1/2)*</td>
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<td>(m<em>x</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,1/2)</td>
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<td>135.7.1149</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/mb'c'</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/m (0,0,0; a,b,c) (1<em>0,0,0) (2</em>z<em>0,0,1/2) (2</em>z<em>1/2,1/2,0) (2</em>y<em>0,0,0) (2</em>x*0,0,0)</td>
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<td>(2<em>x</em>1/2,1/2,2)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,1/2)*</td>
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<td>(m<em>x</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,1/2)</td>
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<td>135.8.1150</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/mb'c'</td>
<td>P&amp;b2 (0,0,1/4; a,b,c) (1<em>0,0,0) (2</em>z<em>0,0,1/2) (2</em>z<em>1/2,1/2,0) (2</em>y<em>0,0,0) (2</em>x*0,0,0)</td>
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<td>(2<em>x</em>1/2,1/2,2)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,1/2)*</td>
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<td></td>
<td></td>
<td>(m<em>x</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,1/2)</td>
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<td>135.9.1151</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt;/mb'c'</td>
<td>P4&lt;sub&gt;2&lt;/sub&gt; 2&lt;sub&gt;1&lt;/sub&gt;2 (1/2,0,1/4; a,b,c) (1<em>0,0,0) (2</em>z<em>0,0,1/2) (2</em>z<em>1/2,1/2,0) (2</em>y<em>0,0,0) (2</em>x*0,0,0)</td>
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<tr>
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<td></td>
<td>(2<em>x</em>1/2,1/2,2)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,0)* (2<em>y</em>1/2,1/2,1/2)*</td>
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<td>(m<em>x</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,0) (m<em>y</em>1/2,1/2,1/2)</td>
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<td>136.1.1152</td>
<td>P4$_2$/mm</td>
<td>(m$<em>x^<em>$$1/2$,1/2,0)' (m$_y^</em>$$1/2$,1/2,0)' (m$</em>{xy}^<em>$$1/2$,1/2,1/2)' (m$_{sy}^</em>$$1/2$,1/2,1/2)'</td>
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<tr>
<td>136.2.1153</td>
<td>P4$_2$/mm1'</td>
<td>(1<em>0,0,0) (4$_z^</em>$$1/2$,1/2,1/2) (2$<em>y^*$$0$,0,0) (4$</em>{sy}^*$$0$,0,0)</td>
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<td>136.3.1154</td>
<td>P4$_2$/m'nm</td>
<td>P4$_2$nm (0,0,0;a,b,c) (4$<em>z^<em>$$1/2$,1/2,1/2) (2$_y^</em>$$0$,0,0) (4$</em>{sy}^*$$0$,0,0)</td>
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<td>136.4.1155</td>
<td>P4$_2$/m'n'm</td>
<td>Cmmm (0,0,0;a-b,a+b,c) (4$<em>z^<em>$$1/2$,1/2,1/2) (2$_y^</em>$$0$,0,0) (4$</em>{sy}^*$$0$,0,0)</td>
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<td>136.5.1156</td>
<td>P4$_2$/m'n'm</td>
<td>Pnnm (0,0,0;a,b,c) (4$<em>z^<em>$$1/2$,1/2,1/2) (2$_y^</em>$$0$,0,0) (4$</em>{sy}^*$$0$,0,0)</td>
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<td>136.6.1157</td>
<td>P4$_2$/m'n'm</td>
<td>P&amp;21m (1/2,0,1/4;a,b,c) (4$<em>z^<em>$$1/2$,1/2,1/2) (2$_y^</em>$$0$,0,0) (4$</em>{sy}^*$$0$,0,0)</td>
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<td>136.7.1158</td>
<td>P4$_2$/mn'm</td>
<td>P4$_2$/m (1/2,0,0;a,b,c) (4$<em>z^<em>$$1/2$,1/2,1/2) (2$_y^</em>$$0$,0,0) (4$</em>{sy}^*$$0$,0,0)</td>
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<td>Magnetic Space Group Elements</td>
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<tr>
<td><strong>136.8.1159</strong> P4₂'/m'n'm' P4₅n2</td>
<td>(1/2,0,1/4;a,b,c)</td>
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<td><strong>137.2.1162</strong> P4₂/nmc1'</td>
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<td><strong>137.3.1163</strong> P4₂/n'mc P4₂,mc</td>
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137.6.1166  P4_2'/n'm'c  P&2_c  (0,0,0;a,b,c)
(2x *1/2,1/2,1/2)  (2y *1/2,1/2,1/2)  (2z *0,0,0)'
(m_x *0,0,0)  (m_y *0,0,0)  (m_z *1/2,1/2,1/2)'

137.7.1167  P4_2/n'm'c'  P4_2/n  (0,0,0;a,b,c)
(2x *1/2,1/2,1/2)  (2y *1/2,1/2,1/2)  (2z *0,0,0)'
(m_x *0,0,0)  (m_y *0,0,0)  (m_z *1/2,1/2,1/2)'

137.8.1168  P4_2'/n'mc'  P&m2  (0,0,0;a,b,c)
(2x *1/2,1/2,1/2)  (2y *1/2,1/2,1/2)  (2z *0,0,0)'
(m_x *0,0,0)  (m_y *0,0,0)  (m_z *1/2,1/2,1/2)'

137.9.1169  P4_2'/n'mc'  P4_2 2,2  (0,0,0;a,b,c)
(2x *1/2,1/2,1/2)  (2y *1/2,1/2,1/2)  (2z *0,0,0)'
(m_x *0,0,0)  (m_y *0,0,0)  (m_z *1/2,1/2,1/2)'

138.1.1170  P4_2/ncm
(2x *1/2,1/2,0)  (2y *1/2,1/2,0)  (2z *0,0,0)'
(m_x *0,0,1/2)  (m_y *0,0,1/2)  (m_z *1/2,1/2,0)'

138.2.1171  P4_2/ncm1'

138.3.1172  P4_2/n'cm  P4_2 cm  (1/2,0,0;a,b,c)
(2x *1/2,1/2,0)  (2y *1/2,1/2,0)  (2z *0,0,1/2)'
(m_x *0,0,0)  (m_y *0,0,0)  (m_z *1/2,1/2,0)'

MAGNETIC SPACE GROUP ELEMENTS 105
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<th>( (m_x,0,1/2) )</th>
<th>( (m_y,0,1/2) )</th>
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MAGNETIC SPACE GROUP ELEMENTS

139.2.1180 I4/mmm1' (0,0,0; a,b,c) (1*0,0,0) (2*0,0,0) (2*0,0,0) (4*0,0,0)
(2x*0,0,0) (2y*0,0,0) (2z*0,0,0) (mz*0,0,0)
(mx*0,0,0) (my*0,0,0) (mz*0,0,0) (mz*0,0,0)

(139.3.1181 I4/m'nm I4mm (0,0,0; a-b,a+b,c) (1*0,0,0) (2*0,0,0) (2*0,0,0) (4*0,0,0)
(2x*0,0,0)' (2y*0,0,0)' (2z*0,0,0)' (mz*0,0,0)' (mz*0,0,0)
(mx*0,0,0) (my*0,0,0) (mz*0,0,0) (mz*0,0,0)

(139.4.1182 I4'/mm' Fmmm (0,0,0; a-b,a+b,c) (1*0,0,0) (2*0,0,0) (2*0,0,0) (4*0,0,0)
(2x*0,0,0)' (2y*0,0,0)' (2z*0,0,0)' (mz*0,0,0)' (mz*0,0,0)
(mx*0,0,0) (my*0,0,0) (mz*0,0,0) (mz*0,0,0)

(139.5.1183 I4'/mmm Immm (0,0,0; a,b,c) (1*0,0,0) (2*0,0,0) (2*0,0,0) (4*0,0,0)
(2x*0,0,0)' (2y*0,0,0)' (2z*0,0,0)' (mz*0,0,0)' (mz*0,0,0)
(mx*0,0,0) (my*0,0,0) (mz*0,0,0) (mz*0,0,0)

(139.6.1184 I4'/m'm'm I&2m (0,0,0; a,b,c) (1*0,0,0) (2*0,0,0) (2*0,0,0) (4*0,0,0)
(2x*0,0,0)' (2y*0,0,0)' (2z*0,0,0)' (mz*0,0,0)' (mz*0,0,0)
(mx*0,0,0) (my*0,0,0) (mz*0,0,0) (mz*0,0,0)

(139.7.1185 I4/m'm'm I4/m (0,0,0; a,b,c) (1*0,0,0) (2*0,0,0) (2*0,0,0) (4*0,0,0)
(2x*0,0,0)' (2y*0,0,0)' (2z*0,0,0)' (mz*0,0,0)' (mz*0,0,0)
(mx*0,0,0) (my*0,0,0) (mz*0,0,0) (mz*0,0,0)

(139.8.1186 I4'/m'm'm I&m2 (0,0,0; a,b,c) (1*0,0,0) (2*0,0,0) (2*0,0,0) (4*0,0,0)
(2x*0,0,0)' (2y*0,0,0)' (2z*0,0,0)' (mz*0,0,0)' (mz*0,0,0)
(mx*0,0,0) (my*0,0,0) (mz*0,0,0) (mz*0,0,0)
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| 140.5.1200 | I4'/mcm' | 1bam | (1/2,0,0; a,b,c) | (1*0,0,0) | (4_z*0,0,0)' | (2_x*0,0,0) | (4_z*1*0,0,0)' |
| 140.6.1201 | I4'/m'c'm | I&2m | (1/2,0,1/4; a,b,c) | (1*0,0,0) | (4_z*0,0,0)' | (2_x*0,0,0) | (4_z*1*0,0,0)' |
| 140.7.1202 | I4/mc'm' | I4/m | (0,0,0; a,b,c) | (1*0,0,0) | (4_z*0,0,0)' | (2_x*0,0,0) | (4_z*1*0,0,0)' |
| 140.8.1203 | I4'/m'cm' | I&c2 | (0,0,0; a,b,c) | (1*0,0,0) | (4_z*0,0,0)' | (2_x*0,0,0) | (4_z*1*0,0,0)' |
| 140.9.1204 | I4/m'c'm' | I422 | (0,0,1/4; a,b,c) | (1*0,0,0) | (4_z*0,0,0)' | (2_x*0,0,0) | (4_z*1*0,0,0)' |
| 140.10.1205 | I_p 4/mcm | P4/mcc | (0,0,0; a,b,c) | (1*0,0,0) | (4_z*0,0,0)' | (2_x*0,0,0) | (4_z*1*0,0,0)' |
| 140.11.1206 | I_p 4/m'cm | P4/ncc | (1/2,0,1/4; a,b,c) | (1*0,0,0) | (4_z*0,0,0)' | (2_x*0,0,0) | (4_z*1*0,0,0)' |

MAGNETIC SPACE GROUP ELEMENTS 110
<p>| 140.12.1207 | I, 4/mcm | P4₂/mbc | (1/2,0,0; a,b,c) | (mₓ<em>0,0,1/2) | (mᵧ</em>0,0,1/2) | (mᵦ<em>0,0,1/2) | (mᵧ</em>0,0,1/2) |
| 140.13.1208 | I, 4/mcm | P4₂/mcm | (1/2,0,0; a,b,c) | (1<em>0,0,0) | (4₁</em>0,1/2,1/2) | (2<em>0,0,0) | (2ₛ</em>0,0,1/2) |
| 140.14.1209 | I, 4/mcm | P4₂/nbc | (0,0,0; a,b,c) | (2<em>0,0,1/2) | (2</em>0,0,1/2) | (2<em>0,0,1/2) | (2ₛ</em>0,0,1/2) |
| 140.15.1210 | I, 4/mcm | P4/mbm | (0,0,0; a,b,c) | (1<em>0,0,0) | (4₁</em>0,1/2,1/2) | (2<em>0,0,0) | (2ₛ</em>0,0,1/2) |
| 140.16.1211 | I, 4/mcm | P4₂/nbm | (0,0,0; a,b,c) | (2<em>0,0,1/2) | (2</em>0,0,1/2) | (2<em>0,0,1/2) | (2ₛ</em>0,0,1/2) |
| 140.17.1212 | I, 4/mcm | P4/nbm | (0,0,1/4; a,b,c) | (1<em>0,0,0) | (4₁</em>0,1/2,1/2) | (2<em>0,0,0) | (2ₛ</em>0,0,1/2) |
| 141.1213 | I4, amd | | | (1<em>0,0,0) | (4₂</em>0,1/2,1/4) | (2<em>0,0,0) | (2ₛ</em>0,0,0) |</p>
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<td>(0,0,0;a,b,c)</td>
<td>(*0,0,0) (4z^*0,1/2,1/4) (m_x^*0,0,0) (m_y^*0,0,0) (m_xy^*0,1/2,1/4) (m_z^*0,0,0)</td>
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<tr>
<td>I4:/a'</td>
<td></td>
<td>(0,0,0; a+b, -a+b, c)</td>
<td>(1<em>0,0,0) (2x</em>0,1/2,1/4)' (m_x<em>0,0,0)' (m_y</em>0,0,0)' (m_z<em>0,1/2,1/4)' (m_z</em>0,1/2,1/4)'</td>
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<tr>
<td>I4'/am'd</td>
<td>Fddd</td>
<td>(0,0,0; c, b, a)</td>
<td>(1<em>0,0,0) (2x</em>0,1/2,1/4)' (m_x<em>0,0,0)' (m_y</em>0,0,0)' (m_z*0,1/2,1/4)'</td>
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<tr>
<td>I4'/a'md'</td>
<td>Imma</td>
<td>(0,1/4,1/8; c, b, a)</td>
<td>(1<em>0,0,0) (2x</em>0,1/2,1/4)' (m_x<em>0,0,0)' (m_y</em>0,0,0)' (m_z*0,1/2,1/4)'</td>
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<tr>
<td>I4'/a'md'</td>
<td>I4/a</td>
<td>(0,0,0; a, b, c)</td>
<td>(1<em>0,0,0) (2x</em>0,1/2,1/4)' (m_x<em>0,0,0)' (m_y</em>0,0,0)' (m_z*0,1/2,1/4)'</td>
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<td>I4'/a'md'</td>
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<td>(1<em>0,0,0) (2x</em>0,1/2,1/4)' (m_x<em>0,0,0)' (m_y</em>0,0,0)' (m_z*0,1/2,1/4)'</td>
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MAGNETIC SPACE GROUP ELEMENTS 113
| 142.7.1228 | I4₁/ac'd' | I4₁/a | (0,0,0; a,b,c) | (1*0,0,0) | (2ₓ*0,1/2,3/4)' | (2ᵧ*0,1/2,3/4)' | (2z*0,0,0) | (4ₓ*0,1/2,1/4) | (4ᵧ*0,1/2,1/4) | (4z*0,1/2,1/4) | (2sₓ*0,0,1/2)' | (2sᵧ*0,0,1/2)' | (2z*1*0,0,0) | (mₓ*0,0,1/2)' | (mᵧ*0,0,1/2)' | (mz*0,1/2,1/4) | (mz*0,1/2,3/4) | (mz*0,1/2,3/4) | (mz*0,0,0) | (mz*0,1/2,3/4) | (mz*0,1/2,3/4) | (mz*0,0,1/2) | (mz*0,0,1/2) | (mz*0,1/2,3/4) | (mz*0,1/2,3/4) |
| 142.8.1229 | I4₁'/a'cd' | I₆c2 | (0,0,0; a,b,c) | (1*0,0,0) | (2ₓ*0,1/2,3/4)' | (2ᵧ*0,1/2,3/4)' | (2z*0,0,0) | (4ₓ*0,1/2,1/4) | (4ᵧ*0,1/2,1/4) | (4z*0,1/2,1/4) | (2sₓ*0,0,1/2) | (2sᵧ*0,0,1/2) | (2z*1*0,0,0) | (mₓ*0,0,1/2)' | (mᵧ*0,0,1/2)' | (mz*0,1/2,1/4) | (mz*0,1/2,3/4) | (mz*0,1/2,3/4) | (mz*0,0,0) | (mz*0,1/2,3/4) | (mz*0,1/2,3/4) |
| 142.9.1230 | I4₁/a'c'd' | I4₂2 | (0,0,1/4; a,b,c) | (1*0,0,0) | (2ₓ*0,1/2,3/4) | (2ᵧ*0,1/2,3/4) | (2z*0,0,0) | (4ₓ*0,1/2,1/4) | (4ᵧ*0,1/2,1/4) | (4z*0,1/2,1/4) | (2sₓ*0,0,1/2) | (2sᵧ*0,0,1/2) | (2z*1*0,0,0) | (mₓ*0,0,1/2)' | (mᵧ*0,0,1/2)' | (mz*0,1/2,1/4) | (mz*0,1/2,3/4) | (mz*0,1/2,3/4) | (mz*0,0,0) | (mz*0,1/2,3/4) | (mz*0,1/2,3/4) |

**TRIGONAL SYSTEM**

| 143.1.1231 | P³ | (1*0,0,0) | (3ₓ*0,0,0) | (3z*1*0,0,0) |
| 143.2.1232 | P3₁' |
| 143.3.1233 | P₂c 3 | P³ | (0,0,0; a,b,2c) | (1*0,0,0) | (3ₓ*0,0,0) | (3z*1*0,0,0) |

<p>| 144.1.1234 | P₃₁ | (1<em>0,0,0) | (3ₓ</em>0,0,1/3) | (3z<em>1</em>0,0,2/3) |
| 144.2.1235 | P₃₁' |
| 144.3.1236 | P₂c 3₂ | P₃₂ | (0,0,0; a,b,2c) | (1<em>0,0,0) | (3ₓ</em>0,0,4/3) | (3z<em>1</em>0,0,2/3) |
| 145.1.1237 | P3₂ | (1<em>0,0,0) | (3₂</em>0,0,2/3) | (3₂⁻¹<em>0,0,1/3) |
| 145.2.1238 | P3₁ | (1</em>0,0,0) | (3₂<em>0,0,2/3) | (3₂⁻¹</em>0,0,4/3) |
| 145.3.1239 | P₂c 3₁ | (0,0,0; a,b,2c) | (1<em>0,0,0) | (3₂</em>0,0,0) | (3₂⁻¹<em>0,0,0) |
| 146.1.1240 | R3 | (1</em>0,0,0) | (3₂<em>0,0,0) | (3₂⁻¹</em>0,0,0) |
| 146.2.1241 | R₃₁' | (1<em>0,0,0) | (3₂</em>0,0,0) | (3₂⁻¹<em>0,0,0) |
| 146.3.1242 | R₆ 3 | (0,0,0; a+b,b+c,a+c) | (1</em>0,0,0) | (3₂<em>0,0,0) | (3₂⁻¹</em>0,0,0) |
| 147.1.1243 | P₆ | (1<em>0,0,0) | (3₂</em>0,0,0) | (3₂⁻¹<em>0,0,0) |
| 147.2.1244 | P₆₁' | (1</em>0,0,0) | (3₂<em>0,0,0) | (3₂⁻¹</em>0,0,0) |
| 147.3.1245 | P₆ | (0,0,0; a,b,c) | (1<em>0,0,0) | (3₂</em>0,0,0) | (3₂⁻¹<em>0,0,0) |
| 147.4.1246 | P₂c₆ | (0,0,0; a,b,2c) | (1</em>0,0,0) | (3₂<em>0,0,0) | (3₂⁻¹</em>0,0,0) |
| 148.1.1247 | R₆ | (1<em>0,0,0) | (3₂</em>0,0,0) | (3₂⁻¹<em>0,0,0) |
| 148.2.1248 | R₆₁' | (1</em>0,0,0) | (3₂<em>0,0,0) | (3₂⁻¹</em>0,0,0) |
| 148.3.1249 | R₆ | (0,0,0; a,b,c) | (1<em>0,0,0) | (3₂</em>0,0,0) | (3₂⁻¹*0,0,0) |</p>
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MAGNETIC SPACE GROUP ELEMENTS 116
151.2.1260  P3\textsubscript{1}121'

151.3.1261  P3\textsubscript{1}12'  P3\textsubscript{1} (0,0,0;a,b,c)  (1\textsuperscript{*}0,0,0)  (2\textsubscript{1}x0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,1/3)  (2\textsubscript{2}x0,0,0,1/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)

151.4.1262  P\textsubscript{2c} \textsubscript{3} 12  P3\textsubscript{1}12 (0,0,0;a,b,2c)  (1\textsuperscript{*}0,0,0)  (2\textsubscript{1}x0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0)\textsuperscript{*} (3\textsubscript{2}x0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)  (3\textsubscript{1}x0,0,0,4/3)  (3\textsubscript{1}x0,0,0,2/3)

152.1.1263  P3\textsubscript{1}21  (1\textsuperscript{*}0,0,0)  (3\textsubscript{1}x0,0,0,1/3)  (3\textsubscript{1}x0,0,0,2/3)

152.2.1264  P3\textsubscript{1}211'  (2\textsuperscript{*}0,0,0,2/3)  (2\textsubscript{1}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,1/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)

152.3.1265  P3\textsubscript{1}2'1  P3\textsubscript{1} (0,0,0;a,b,c)  (1\textsuperscript{*}0,0,0)  (2\textsubscript{1}x0,0,0,2/3)\textsuperscript{*} (2\textsubscript{1}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,1/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)

152.4.1266  P\textsubscript{2c} \textsubscript{2} 121  P3\textsubscript{1}21 (0,0,0;a,b,2c)  (1\textsuperscript{*}0,0,0)  (2\textsubscript{1}x0,0,0,2/3)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)

153.1.1267  P3\textsubscript{2}12  (1\textsuperscript{*}0,0,0)  (3\textsubscript{1}x0,0,0,2/3)  (3\textsubscript{2}x0,0,0,1/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,1/3)

153.2.1268  P3\textsubscript{2}121'  (2\textsuperscript{*}0,0,0,2/3)  (2\textsubscript{1}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,1/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)

153.3.1269  P3\textsubscript{2}12'  P3\textsubscript{2} (0,0,0;a,b,c)  (1\textsuperscript{*}0,0,0)  (2\textsubscript{1}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,1/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,2/3)\textsuperscript{*} (3\textsubscript{1}x0,0,0,1/3)

153.4.1270  P\textsubscript{2c} \textsubscript{3} 12  P3\textsubscript{1}12 (0,0,0;a,b,2c)  (1\textsuperscript{*}0,0,0)  (2\textsubscript{1}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (2\textsubscript{2}x0,0,0,0)\textsuperscript{*} (3\textsubscript{1}x0,0,0,4/3)  (3\textsubscript{1}x0,0,0,2/3)  (3\textsubscript{1}x0,0,0,2/3)
<p>| Magnetic Space Group Elements |elm| |elm| |elm| |
|-----------------------------|----|---|---|---|---|
| 154.1.1271 P32 21 | (1<em>0,0,0) | (3z</em>0,0,2/3) | (3z-1<em>0,0,1/3) |
| 154.2.1272 P32 211' | (2x</em>0,0,1/3) | (2xy<em>0,0,0) | (2y</em>0,0,2/3) |
| 154.3.1273 P32 2'1 P3 | (1<em>0,0,0) | (3z</em>0,0,2/3) | (3z-1<em>0,0,1/3) |
| 154.4.1274 P2c 3,21 P3121 | (2x</em>0,0,1/3) | (2xy<em>0,0,0) | (2y</em>0,0,2/3) |
| 155.1.1275 R32 | (1<em>0,0,0) | (3z</em>0,0,0) | (3z-1<em>0,0,0) |
| 155.2.1276 R321' | (2x</em>0,0,0) | (2xy<em>0,0,0) | (2y</em>0,0,0) |
| 155.3.1277 R32' R3 | (1<em>0,0,0) | (3z</em>0,0,0) | (3z-1<em>0,0,0) |
| 155.4.1278 R3 32 | (2x</em>0,0,0) | (2xy<em>0,0,0) | (2y</em>0,0,0) |
| 156.1.1279 P3m1 | (1<em>0,0,0) | (3z</em>0,0,0) | (3z-1<em>0,0,0) |
| 156.2.1280 P3m11' | (mx</em>0,0,0) | (mxy<em>0,0,0) | (my</em>0,0,0) |
| 156.3.1281 P3m1' P3 | (1<em>0,0,0) | (3z</em>0,0,0) | (3z-1<em>0,0,0) |
|                     | (mx</em>0,0,0)' | (mxy<em>0,0,0)' | (my</em>0,0,0)' |</p>
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163.2.1311  P&1c1'

163.3.1312  P&'1c  P31c  (0, 0, 0; a, b, c) | (1, 0, 0, 0) | (3, 0, 0, 0) | (3, -1, 0, 0, 0) |
|           | (m, 0, 0, 1/2) | (m, 0, 0, 1/2) | (m, 0, 0, 1/2) |
|           | (2, 0, 0, 1/2) | (2, 0, 0, 1/2) | (2, 0, 0, 1/2) |

163.4.1313  P&'1c'  P312  (0, 0, 1/4; a, b, c) | (1, 0, 0, 0) | (3, 0, 0, 0) | (3, -1, 0, 0, 0) |
|           | (m, 0, 0, 1/2) | (m, 0, 0, 1/2) | (m, 0, 0, 1/2) |
|           | (2, 0, 0, 1/2) | (2, 0, 0, 1/2) | (2, 0, 0, 1/2) |

163.5.1314  P&1c'  P&  (0, 0, 0; a, b, c) | (1, 0, 0, 0) | (3, 0, 0, 0) | (3, -1, 0, 0, 0) |
|           | (m, 0, 0, 1/2) | (m, 0, 0, 1/2) | (m, 0, 0, 1/2) |
|           | (2, 0, 0, 1/2) | (2, 0, 0, 1/2) | (2, 0, 0, 1/2) |

164.1.1315  P&m1 | (1, 0, 0, 0) | (3, 0, 0, 0) | (3, -1, 0, 0, 0) |
|           | (m, 0, 0, 0) | (m, 0, 0, 0) | (m, 0, 0, 0) |
|           | (2, 0, 0, 0) | (2, 0, 0, 0) | (2, 0, 0, 0) |

164.2.1316  P&m11' |

164.3.1317  P&m1  P3m1  (0, 0, 0; a, b, c) | (1, 0, 0, 0) | (3, 0, 0, 0) | (3, -1, 0, 0, 0) |
<p>|           | (m, 0, 0, 0) | (m, 0, 0, 0) | (m, 0, 0, 0) |
|           | (2, 0, 0, 0) | (2, 0, 0, 0) | (2, 0, 0, 0) |</p>
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</table>
165.4.1325  P&'c'1  P321  (0,0,1/4;a,b,c)  
(2x*0,0,1/2)'  (2xy*0,0,1/2)'  (2y*0,0,1/2)'
(1*0,0,0)  (3,0,0,0)  (3,-1*0,0,0)
(&*0,0,0)'  (&z*0,0,0)'  (&z,-1*0,0,0)'
(mx*0,0,1/2)'  (mxy*0,0,1/2)'  (my*0,0,1/2)'
(2x*0,0,1/2)  (2xy*0,0,1/2)  (2y*0,0,1/2)

165.5.1326  P&c'1  P&  (0,0,0;a,b,c)  
(1*0,0,0)  (3,0,0,0)  (3,-1*0,0,0)
(&*0,0,0)  (&z*0,0,0)  (&z,-1*0,0,0)
(mx*0,0,1/2)'  (mxy*0,0,1/2)'  (my*0,0,1/2)'
(2x*0,0,1/2)'  (2xy*0,0,1/2)'  (2y*0,0,1/2)'

166.1.1327  R&'m  
(1*0,0,0)  (3,0,0,0)  (3,-1*0,0,0)
(&*0,0,0)  (&z*0,0,0)  (&z,-1*0,0,0)
(mx*0,0,0)  (mxy*0,0,0)  (my*0,0,0)
(2x*0,0,0)  (2xy*0,0,0)  (2y*0,0,0)

166.2.1328  R&'m1'  

166.3.1329  R&'m  R3m  (0,0,0;a,b,c)  
(1*0,0,0)  (3,0,0,0)  (3,-1*0,0,0)
(&*0,0,0)'  (&z*0,0,0)'  (&z,-1*0,0,0)'
(mx*0,0,0)  (mxy*0,0,0)  (my*0,0,0)
(2x*0,0,0)'  (2xy*0,0,0)'  (2y*0,0,0)'

166.4.1330  R&'m'  R32  (0,0,0;a,b,c)  
(1*0,0,0)  (3,0,0,0)  (3,-1*0,0,0)
(&*0,0,0)'  (&z*0,0,0)'  (&z,-1*0,0,0)'
(mx*0,0,0)'  (mxy*0,0,0)'  (my*0,0,0)'
(2x*0,0,0)  (2xy*0,0,0)  (2y*0,0,0)

166.5.1331  R&'m'  R&  (0,0,0;a,b,c)  
(1*0,0,0)  (3,0,0,0)  (3,-1*0,0,0)
(&*0,0,0)  (&z*0,0,0)  (&z,-1*0,0,0)
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<th>Magnetic Space Group Elements</th>
<th>R &amp; m</th>
<th>(0,0,0;a+b,b+c,a+c)</th>
<th>(m_x*0,0,0)'</th>
<th>(m_y*0,0,0)'</th>
<th>(m_z*0,0,0)'</th>
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<tbody>
<tr>
<td>166.6.1332</td>
<td>R &amp; m</td>
<td>(0,0,0;a+b,b+c,a+c)</td>
<td>(1*0,0,0)</td>
<td>(3_z*0,0,0)</td>
<td>(3_z<em>1</em>0,0,0)</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(2_x*0,0,0)'</td>
<td>(2_xy*0,0,0)'</td>
<td>(2_y*0,0,0)'</td>
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<tr>
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<th>R &amp; m'</th>
<th>(0,0,0;a+b,b+c,a+c)</th>
<th>(m_x*0,0,1)</th>
<th>(m_y*0,0,1)</th>
<th>(m_z*0,0,1)</th>
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<tr>
<td>166.7.1333</td>
<td>R &amp; c</td>
<td>(0,0,0;a+b,b+c,a+c)</td>
<td>(1*0,0,0)</td>
<td>(3_z*0,0,0)</td>
<td>(3_z<em>1</em>0,0,0)</td>
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<td></td>
<td>(2_x*0,0,1/2)</td>
<td>(2_xy*0,0,1/2)</td>
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<table>
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<tr>
<th>Magnetic Space Group Elements</th>
<th>R &amp; c</th>
<th>(0,0,0;a+b,b+c,a+c)</th>
<th>(1*0,0,0)</th>
<th>(3_z*0,0,0)</th>
<th>(3_z<em>1</em>0,0,0)</th>
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<tr>
<td>167.1.1334</td>
<td>R &amp; c</td>
<td>(0,0,0;a,b,c)</td>
<td>(1*0,0,0)</td>
<td>(3_z*0,0,0)</td>
<td>(3_z<em>1</em>0,0,0)</td>
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<td></td>
<td>(2_x*0,0,1/2)</td>
<td>(2_xy*0,0,1/2)</td>
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<tr>
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<th>R &amp; c'</th>
<th>(0,0,1/4;a,b,c)</th>
<th>(1*0,0,0)</th>
<th>(3_z*0,0,0)</th>
<th>(3_z<em>1</em>0,0,0)</th>
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<td>167.4.1337</td>
<td>R &amp; c'</td>
<td>(0,0,0; a,b,c)</td>
<td>(1*0,0,0)</td>
<td>(3_z*0,0,0)</td>
<td>(3_z<em>1</em>0,0,0)</td>
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<td>(2_x*0,0,1/2)</td>
<td>(2_xy*0,0,1/2)</td>
<td>(2_y*0,0,1/2)</td>
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<tr>
<th>Magnetic Space Group Elements</th>
<th>R &amp; c'</th>
<th>(0,0,0; a,b,c)</th>
<th>(1*0,0,0)</th>
<th>(3_z*0,0,0)</th>
<th>(3_z<em>1</em>0,0,0)</th>
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<tr>
<td>167.5.1338</td>
<td>R &amp; c'</td>
<td>(0,0,0; a,b,c)</td>
<td>(1*0,0,0)</td>
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<td>(3_z<em>1</em>0,0,0)</td>
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**HEXAGONAL SYSTEM**

<p>| 168.1.1339 | P6 | (1<em>0,0,0) | (3</em>0,0,0) | (3,-1<em>0,0,0) |
|  |  | (2</em>0,0,0) | (6<em>0,0,0) | (6,-1</em>0,0,0) |
| 168.2.1340 | P61' |  |  |  |
| 168.3.1341 | P6' P3 | (0,0,0; a,b,c) | (1<em>0,0,0) | (3</em>0,0,0) | (3,-1<em>0,0,0) |
|  |  |  | (2</em>0,0,0) | (6<em>0,0,0) | (6,-1</em>0,0,0) |
| 168.4.1342 | P₂c 6 | (0,0,0; a,b,2c) | (1<em>0,0,0) | (3</em>0,0,0) | (3,-1<em>0,0,0) |
|  |  |  | (2</em>0,0,0) | (6<em>0,0,0) | (6,-1</em>0,0,0) |
| 168.5.1343 | P₂c 6' P6₃ | (0,0,0; a,b,2c) | (1<em>0,0,0) | (3</em>0,0,0) | (3,-1<em>0,0,0) |
|  |  |  | (2</em>0,0,1) | (6<em>0,0,1) | (6,-1</em>0,0,1) |
| 169.1.1344 | P₆₁ | (1<em>0,0,0) | (3</em>0,0,1/3) | (3,-1<em>0,0,2/3) |
|  |  | (2</em>0,0,1/2) | (6<em>0,0,1/6) | (6,-1</em>0,0,5/6) |
| 169.2.1345 | P₆₁,1' |  |  |  |
| 169.3.1346 | P₆₁ P3₁ | (0,0,0; a,b,c) | (1<em>0,0,0) | (3</em>0,0,1/3) | (3,-1*0,0,2/3) |</p>
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<td><strong>170.1.1347</strong> P6_5</td>
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<td><strong>170.2.1348</strong> P6_5'</td>
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<td><strong>170.3.1349</strong> P6_5' P3_2</td>
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<td><strong>171.1.1350</strong> P6_2</td>
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<td><strong>171.2.1351</strong> P6_2'</td>
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<tr>
<td><strong>171.3.1352</strong> P6_2' P3_2</td>
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<tr>
<td><strong>171.4.1353</strong> P_2c 6_2 P6_1</td>
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<td><strong>171.5.1354</strong> P_2c 6_2' P6_4</td>
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<td><strong>172.2.1356</strong> P6_4'</td>
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<td><strong>172.3.1357</strong> P6_4' P3_1</td>
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MAGNETIC SPACE GROUP ELEMENTS 127
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<th>1358</th>
<th>P2c 6_4</th>
<th>P6_2</th>
<th>(0,0,0;a,b,2c)</th>
<th>(1<em>0,0,0) (2</em>0,0,0) (6*0,0,2/3) (6^{-1}*0,0,1/3)</th>
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<td>P2c 6'_4</td>
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<td>Code</td>
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<td>P6_3</td>
<td>(0,0,0;0,a,b,c)</td>
<td>(1<em>0,0,0) (2</em>0,0,1/2) (6*0,0,1/2) (6^{-1}*0,0,1/2)</td>
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<td>P6_3</td>
<td>(0,0,0;0,a,b,c)</td>
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<tr>
<td>Code</td>
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<td>P6_3</td>
<td>(0,0,0;0,a,b,c)</td>
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<tr>
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<td>1363</td>
<td>P6_3</td>
<td>(0,0,0;0,a,b,c)</td>
<td>(1<em>0,0,0) (2</em>0,0,1/2) (6*0,0,1/2) (6^{-1}*0,0,1/2)</td>
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<tr>
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<td>P6_3</td>
<td>(0,0,0;0,a,b,c)</td>
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<tr>
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<td>P6_3</td>
<td>(0,0,0;0,a,b,c)</td>
<td>(1<em>0,0,0) (2</em>0,0,1/2) (6*0,0,1/2) (6^{-1}*0,0,1/2)</td>
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<tr>
<td>Code</td>
<td>1366</td>
<td>P6_3</td>
<td>(0,0,0;0,a,b,c)</td>
<td>(1<em>0,0,0) (2</em>0,0,1/2) (6*0,0,1/2) (6^{-1}*0,0,1/2)</td>
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<tr>
<td>Code</td>
<td>1367</td>
<td>P6/m</td>
<td>(1<em>0,0,0) (3</em>0,0,0) (3^{-1}<em>0,0,0) (3</em>0,0,0)</td>
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<tr>
<td>Code</td>
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<td>(6<em>0,0,0) (6</em>0,0,0) (6<em>0,0,0) (6</em>0,0,0)</td>
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MAGNETIC SPACE GROUP ELEMENTS 128
<table>
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<th>Elements</th>
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</table>
| 175.2.1368 P6/m1'   | $\begin{array}{ccc}
(2z,0,0,0) & (6z,0,0,0) & (6z^{-1},0,0,0) \\
(mz,0,0,0) & (6z,0,0,0) & (6z^{-1},0,0,0)
\end{array}$ |
| 175.3.1369 P6'/m    | $\begin{array}{ccc}
(1z,0,0,0) & (3z,0,0,0) & (3z^{-1},0,0,0) \\
(&z,0,0,0)' & (6z,0,0,0) & (6z^{-1},0,0,0)
\end{array}$ |
| 175.4.1370 P6/m'    | $\begin{array}{ccc}
(1z,0,0,0) & (3z,0,0,0) & (3z^{-1},0,0,0) \\
(&z,0,0,0)' & (6z,0,0,0) & (6z^{-1},0,0,0)
\end{array}$ |
| 175.5.1371 P6'/m'   | $\begin{array}{ccc}
(1z,0,0,0) & (3z,0,0,0) & (3z^{-1},0,0,0) \\
(&z,0,0,0)' & (6z,0,0,0) & (6z^{-1},0,0,0)
\end{array}$ |
| 175.6.1372 P2c 6/m  | $\begin{array}{ccc}
(1z,0,0,0) & (3z,0,0,0) & (3z^{-1},0,0,0) \\
(&z,0,0,0)' & (6z,0,0,0) & (6z^{-1},0,0,0)
\end{array}$ |
| 175.7.1373 P2c 6'/m | $\begin{array}{ccc}
(1z,0,0,0) & (3z,0,0,0) & (3z^{-1},0,0,0) \\
(&z,0,0,1) & (6z,0,0,1) & (6z^{-1},0,0,1)
\end{array}$ |
| 176.1.1374 P63/m    | $\begin{array}{ccc}
(1z,0,0,0) & (3z,0,0,0) & (3z^{-1},0,0,0)
\end{array}$ |
(0,0,0) (3,-1*0,0,0) (6,-1*0,0,0)
(2,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)
(m,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)

176.2.1375 P6$_3$/m1'

176.3.1376 P6$_3$'/m P& (0,0,1/4;a,b,c) (1*0,0,0) (3,-1*0,0,0) (3,-1*0,0,0)
(6,-1*0,0,0) (6,-1*0,0,0) (6,-1*0,0,0)
(2,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)
(m,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)

176.4.1377 P6$_3$/m' P6$_3$ (0,0,0;a,b,c) (1*0,0,0) (3,-1*0,0,0) (3,-1*0,0,0)
(6,-1*0,0,0) (6,-1*0,0,0) (6,-1*0,0,0)
(2,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)
(m,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)

176.5.1378 P6$_3$'/m' P& (0,0,0;a,b,c) (1*0,0,0) (3,-1*0,0,0) (3,-1*0,0,0)
(6,-1*0,0,0) (6,-1*0,0,0) (6,-1*0,0,0)
(2,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)
(m,-1*0,0,1/2) (6,-1*0,0,1/2) (6,-1*0,0,1/2)

177.1.1379 P622 (1*0,0,0) (3,-1*0,0,0) (3,-1*0,0,0)
(2,-1*0,0,0) (6,-1*0,0,0) (6,-1*0,0,0)
(2,-1*0,0,0) (2,-1*0,0,0) (2,-1*0,0,0)

177.2.1380 P6221'

177.3.1381 P6'2'2 P312 (0,0,0;a,b,c) (1*0,0,0) (3,-1*0,0,0) (3,-1*0,0,0)
(2,-1*0,0,0) (6,-1*0,0,0) (6,-1*0,0,0)
(2,-1*0,0,0) (2,-1*0,0,0) (2,-1*0,0,0)
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**MAGNETIC SPACE GROUP ELEMENTS 131**
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<td>180.2.1397</td>
<td>P6(_2)221'</td>
<td>((1^*0,0,0))  ((3^*0,0,2/3))  ((3^*1^*0,0,1/3))  ((2^*0,0,0))  ((6^*0,0,1/3))  ((6^*1^*0,0,2/3))  ((2^*0,0,1/3))  ((2^*0,0,0))  ((2^*0,0,2/3))</td>
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</tr>
<tr>
<td>180.3.1398</td>
<td>P6(_2)'2'2</td>
<td>((0,0,1/6;a,b,c))  ((1^*0,0,0))  ((3^*0,0,2/3))  ((3^*1^*0,0,1/3))  ((2^*0,0,0))  ((6^*0,0,1/3))  ((6^*1^*0,0,2/3))  ((2^*0,0,1/3))  ((2^*0,0,0))  ((2^*0,0,2/3))</td>
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<tr>
<td>180.4.1399</td>
<td>P6(_2)'2'2</td>
<td>((0,0,-1/6;a,b,c))  ((1^*0,0,0))  ((3^*0,0,2/3))  ((3^*1^*0,0,1/3))  ((2^*0,0,0))  ((6^*0,0,1/3))  ((6^*1^*0,0,2/3))  ((2^*0,0,1/3))  ((2^*0,0,0))  ((2^*0,0,2/3))</td>
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<tr>
<td>180.5.1400</td>
<td>P6(_2)'2'2</td>
<td>((0,0,0;a,b,c))  ((1^*0,0,0))  ((3^*0,0,2/3))  ((3^*1^*0,0,1/3))  ((2^*0,0,0))  ((6^*0,0,1/3))  ((6^*1^*0,0,2/3))  ((2^*0,0,1/3))  ((2^*0,0,0))  ((2^*0,0,2/3))</td>
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<tr>
<td>180.6.1401</td>
<td>P(_2c)6(_2)22</td>
<td>((0,0,0;a,b,2c))  ((1^*0,0,0))  ((3^*0,0,2/3))  ((3^*1^*0,0,1/3))  ((2^*0,0,0))  ((6^*0,0,1/3))  ((6^*1^*0,0,2/3))  ((2^*0,0,1/3))  ((2^*0,0,0))  ((2^*0,0,2/3))</td>
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<tr>
<td>180.7.1402</td>
<td>P(_2c)6(_2)'22'</td>
<td>((0,0,0;a,b,2c))  ((1^*0,0,0))  ((3^*0,0,2/3))  ((3^*1^*0,0,1/3))  ((2^*0,0,0))  ((6^*0,0,1/3))  ((6^*1^*0,0,2/3))  ((2^*0,0,1/3))  ((2^*0,0,0))  ((2^*0,0,2/3))</td>
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<tr>
<td>181.1.1403</td>
<td>$P_6_{4}22$</td>
<td>$(1*0,0,0)$</td>
<td>$(3_z*0,0,1/3)$</td>
<td>$(3_z^{-1}*0,0,2/3)$</td>
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<tr>
<td>181.2.1404</td>
<td>$P_6_{4}221'$</td>
<td>$(2_z*0,0,0)$</td>
<td>$(6_z*0,0,2/3)$</td>
<td>$(6_z^{-1}*0,0,1/3)$</td>
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<tr>
<td>181.3.1405</td>
<td>$P_6_{4}'2'2$</td>
<td>$(2_x*0,0,0)$</td>
<td>$(2_{xy}*0,0,1/3)$</td>
<td>$(2_{x}^{-1}*0,0,2/3)$</td>
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<tr>
<td>181.4.1406</td>
<td>$P_6_{4}'2'2'$</td>
<td>$(2_y*0,0,0)$</td>
<td>$(2_{y}^{-1}*0,0,1/3)$</td>
<td>$(2_{y}^{-1}*0,0,2/3)$</td>
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<tr>
<td>181.5.1407</td>
<td>$P_6_{4}2'2'$</td>
<td>$(2_1*0,0,0)$</td>
<td>$(2_{2}^{-1}*0,0,0)$</td>
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<tr>
<td>181.6.1408</td>
<td>$P_{2c}6_{4}22$</td>
<td>$(2_1*0,0,0)$</td>
<td>$(2_1^{-1}*0,0,2/3)$</td>
<td>$(2_1^{-1}*0,0,4/3)$</td>
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<tr>
<td>181.7.1409</td>
<td>$P_{2c}6_{4}'2'2'$</td>
<td>$(2_1*0,0,0)$</td>
<td>$(2_1^{-1}*0,0,2/3)$</td>
<td>$(2_1^{-1}*0,0,4/3)$</td>
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</tbody>
</table>

**MAGNETIC SPACE GROUP ELEMENTS 134**
182.1.1410 p6\textsubscript{3} 22
(1\*0,0,0) (3\*0,0,0) (3\*-1\*0,0,0) \\
(2\*0,0,1/2) (6\*0,0,1/2) (6\*-1\*0,0,1/2) \\
(2\*0,0,0) (2\*0,0,0) (2\*0,0,0) \\
(2\*0,0,1/2) (2\*0,0,1/2) (2\*0,0,1/2) \\

182.2.1411 p6\textsubscript{3} 221'

182.3.1412 p6\textsubscript{3}'2'2 P312 (0,0,1/4;a,b,c) (1\*0,0,0) (3\*0,0,0) (3\*-1\*0,0,0) \\
(2\*0,0,1/2)' (6\*0,0,1/2)' (6\*-1\*0,0,1/2)' \\
(2\*0,0,0)' (2\*0,0,0)' (2\*0,0,0)' \\
(2\*0,0,1/2)' (2\*0,0,1/2) (2\*0,0,1/2) \\

182.4.1413 p6\textsubscript{3}'2'2' P321 (0,0,0;a,b,c) (1\*0,0,0) (3\*0,0,0) (3\*-1\*0,0,0) \\
(2\*0,0,1/2)' (6\*0,0,1/2)' (6\*-1\*0,0,1/2)' \\
(2\*0,0,0) (2\*0,0,0) (2\*0,0,0) \\
(2\*0,0,1/2)' (2\*0,0,1/2)' (2\*0,0,1/2) \\

182.5.1414 p6\textsubscript{3}'2'2' P6\textsubscript{3} (0,0,0;a,b,c) (1\*0,0,0) (3\*0,0,0) (3\*-1\*0,0,0) \\
(2\*0,0,1/2) (6\*0,0,1/2) (6\*-1\*0,0,1/2) \\
(2\*0,0,0) (2\*0,0,0) (2\*0,0,0) \\
(2\*0,0,1/2)' (2\*0,0,1/2)' (2\*0,0,1/2) \\

183.1.1415 p6mm (1\*0,0,0) (3\*0,0,0) (3\*-1\*0,0,0) \\
(2\*0,0,0) (6\*0,0,0) (6\*-1\*0,0,0) \\
(m\*0,0,0) (m\*0,0,0) (m\*0,0,0) \\
(m\*0,0,0) (m\*0,0,0) (m\*0,0,0) \\

183.2.1416 P6mm1' 

183.3.1417 P6'm'm P31m (0,0,0;a,b,c) (1\*0,0,0) (3\*0,0,0) (3\*-1\*0,0,0) \\
(2\*0,0,0)' (6\*0,0,0)' (6\*-1\*0,0,0)' \\

MAGNETIC SPACE GROUP ELEMENTS 135
<table>
<thead>
<tr>
<th>Group</th>
<th>Symbol</th>
<th>Cell Parameters</th>
<th>Magnetic Elements</th>
</tr>
</thead>
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<tr>
<td>183.4.1418</td>
<td>P6'mm'</td>
<td>(0,0,0; a,b,c)</td>
<td>( (m_x^0,0,0)' ) (( m_y^0,0,0)' ) (( m_z^0,0,0)' )</td>
</tr>
<tr>
<td>183.5.1419</td>
<td>P6m'm'</td>
<td>(0,0,0; a,b,c)</td>
<td>( (1^*0,0,0) )  (( 2z^*0,0,0) ) (( 3z^*0,0,0)' )</td>
</tr>
<tr>
<td>183.6.1420</td>
<td>P(_2_c_6)mm</td>
<td>(0,0,0; a,b,c)</td>
<td>( (1^*0,0,0) )  (( 2z^*0,0,0) ) (( 3z^*0,0,0)' )</td>
</tr>
<tr>
<td>183.7.1421</td>
<td>P(_2_c_6)mm'</td>
<td>(0,0,0; a,b,2c)</td>
<td>( (1^*0,0,0) )  (( 2z^*0,0,0) ) (( 3z^*0,0,0)' )</td>
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<tr>
<td>183.8.1422</td>
<td>P(_2_c_6)mm'</td>
<td>(0,0,0; a,b,2c)</td>
<td>( (1^*0,0,0) )  (( 2z^*0,0,0) ) (( 3z^*0,0,0)' )</td>
</tr>
<tr>
<td>183.9.1423</td>
<td>P(_2_c_6)m'm'</td>
<td>(0,0,0; a,b,2c)</td>
<td>( (1^*0,0,0) )  (( 2z^*0,0,0) ) (( 3z^*0,0,0)' )</td>
</tr>
<tr>
<td>184.1.1424</td>
<td>P6cc</td>
<td>((1*0,0,0))</td>
<td>((3_z*0,0,0))</td>
</tr>
<tr>
<td>184.1.1424</td>
<td>P6cc</td>
<td>((2_z*0,0,0))</td>
<td>((6_z*0,0,0))</td>
</tr>
<tr>
<td>184.1.1424</td>
<td>P6cc</td>
<td>((m_x*0,0,1/2))</td>
<td>((m_{xy}*0,0,1/2))</td>
</tr>
<tr>
<td>184.1.1424</td>
<td>P6cc</td>
<td>((m_1*0,0,1/2))</td>
<td>((m_2*0,0,1/2))</td>
</tr>
</tbody>
</table>

| 184.2.1425 | P6cc' | \((0,0,0;a,b,c)\) |
| 184.2.1425 | P6cc' | \((1*0,0,0)\) | \((3_z*0,0,0)\) | \((3_z^{-1}*0,0,0)\) |
| 184.2.1425 | P6cc' | \((2_z*0,0,0)'\) | \((6_z*0,0,0)'\) | \((6_z^{-1}*0,0,0)'\) |
| 184.2.1425 | P6cc' | \((m_x*0,0,1/2)'\) | \((m_{xy}*0,0,1/2)'\) | \((m_y*0,0,1/2)'\) |
| 184.2.1425 | P6cc' | \((m_1*0,0,1/2)'\) | \((m_2*0,0,1/2)'\) | \((m_3*0,0,1/2)'\) |

| 184.3.1426 | P6'c\('c\) | P31c | \((0,0,0;a,b,c)\) |
| 184.3.1426 | P6'c\('c\) | P31c | \((1*0,0,0)\) | \((3_z*0,0,0)\) | \((3_z^{-1}*0,0,0)\) |
| 184.3.1426 | P6'c\('c\) | P31c | \((2_z*0,0,0)'\) | \((6_z*0,0,0)'\) | \((6_z^{-1}*0,0,0)'\) |
| 184.3.1426 | P6'c\('c\) | P31c | \((m_x*0,0,1/2)'\) | \((m_{xy}*0,0,1/2)'\) | \((m_y*0,0,1/2)'\) |
| 184.3.1426 | P6'c\('c\) | P31c | \((m_1*0,0,1/2)'\) | \((m_2*0,0,1/2)'\) | \((m_3*0,0,1/2)'\) |

| 184.4.1427 | P6'cc\('c'\) | P3c1 | \((0,0,0;a,b,c)\) |
| 184.4.1427 | P6'cc\('c'\) | P3c1 | \((1*0,0,0)\) | \((3_z*0,0,0)\) | \((3_z^{-1}*0,0,0)\) |
| 184.4.1427 | P6'cc\('c'\) | P3c1 | \((2_z*0,0,0)'\) | \((6_z*0,0,0)'\) | \((6_z^{-1}*0,0,0)'\) |
| 184.4.1427 | P6'cc\('c'\) | P3c1 | \((m_x*0,0,1/2)'\) | \((m_{xy}*0,0,1/2)'\) | \((m_y*0,0,1/2)'\) |
| 184.4.1427 | P6'cc\('c'\) | P3c1 | \((m_1*0,0,1/2)'\) | \((m_2*0,0,1/2)'\) | \((m_3*0,0,1/2)'\) |

| 184.5.1428 | P6c'c\('c'\) | P6 | \((0,0,0;a,b,c)\) |
| 184.5.1428 | P6c'c\('c'\) | P6 | \((1*0,0,0)\) | \((3_z*0,0,0)\) | \((3_z^{-1}*0,0,0)\) |
| 184.5.1428 | P6c'c\('c'\) | P6 | \((2_z*0,0,0)'\) | \((6_z*0,0,0)'\) | \((6_z^{-1}*0,0,0)'\) |
| 184.5.1428 | P6c'c\('c'\) | P6 | \((m_x*0,0,1/2)'\) | \((m_{xy}*0,0,1/2)'\) | \((m_y*0,0,1/2)'\) |
| 184.5.1428 | P6c'c\('c'\) | P6 | \((m_1*0,0,1/2)'\) | \((m_2*0,0,1/2)'\) | \((m_3*0,0,1/2)'\) |

| 185.1.1429 | P6\(_3\) cm | \((0,0,0;a,b,c)\) |
| 185.1.1429 | P6\(_3\) cm | \((1*0,0,0)\) | \((3_z*0,0,0)\) | \((3_z^{-1}*0,0,0)\) |
| 185.1.1429 | P6\(_3\) cm | \((2_z*0,0,0)'\) | \((6_z*0,0,0)'\) | \((6_z^{-1}*0,0,0)'\) |
| 185.1.1429 | P6\(_3\) cm | \((m_x*0,0,1/2)'\) | \((m_{xy}*0,0,1/2)'\) | \((m_y*0,0,1/2)'\) |
| 185.1.1429 | P6\(_3\) cm | \((m_1*0,0,0)'\) | \((m_2*0,0,0)'\) | \((m_3*0,0,0)'\) |

| 185.2.1430 | P6\(_3\) cm'1' | \((0,0,0;a,b,c)\) |
| 185.3.1431 | P6\(_3\) c'm | P312 | \((1*0,0,0)\) | \((3_z*0,0,0)\) | \((3_z^{-1}*0,0,0)\) |
| Magnetic Space Group | Elements | Point Group | |
|----------------------|----------|-------------|
| (2z*0,0,1/2)'       | (3z*0,0,0) | P3c1        |
| (m_x*0,0,1/2)'      | (m_y*0,0,0) | (1*0,0,0)   |
| (m_z*0,0,0)         | (m_z*0,0,0) | (1*0,0,0)   |
|                      |           | (6z*0,0,1/2)' | (3z*0,0,0) |
|                      |           | (m_z*0,0,0) | (m_z*0,0,0) |
|                      |           | (6z*0,0,1/2)' | (3z*0,0,0) |
|                      |           | (m_z*0,0,0) | (m_z*0,0,0) |

185.4.1432 P6_3'cm' P3c1 (0,0,0;a,b,c)

185.5.1433 P6_3 c'm' P6_3 (0,0,0;a,b,c)

186.1.1434 P6_3 mc

186.2.1435 P6_3 mc1'

186.3.1436 P6_3'mc' P31c (0,0,0;a,b,c)

186.4.1437 P6_3'mc' P3m1 (0,0,0;a,b,c)

186.5.1438 P6_3 m'c' P6_3 (0,0,0;a,b,c)
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<td>(2,0,0,1/2)</td>
<td>(6,0,0,1/2)</td>
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<td>(m*,0,0,0)'</td>
<td>(m*,0,0,0)'</td>
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<tr>
<td>(m*,0,1/2)'</td>
<td>(m*,0,1/2)'</td>
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<td>(187.1.1439 P6m2)</td>
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<td>(3,-1*,0,0,0)</td>
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<tr>
<td>(m*,0,0,0)</td>
<td>(6*,0,0,0)</td>
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<tr>
<td>(m*,0,0,0)'</td>
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<tr>
<td>(m*,0,1/2)'</td>
<td>(6*,0,1/2)'</td>
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<td>(187.2.1440 P6m2')</td>
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<td>(2,0,0,0)</td>
<td>(2,0,0,0)</td>
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<td>(187.3.1441 P6m') P312</td>
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<td>(1*,0,0,0)</td>
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<tr>
<td>(3,0,0,0)</td>
<td>(3,-1*,0,0,0)</td>
</tr>
<tr>
<td>(m*,0,0,0)</td>
<td>(6*,0,0,0)</td>
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<tr>
<td>(m*,0,0,0)'</td>
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<tr>
<td>(m*,0,1/2)'</td>
<td>(6*,0,1/2)'</td>
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<tr>
<td>(m*,0,0,0)</td>
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<td>(m*,0,0,0)'</td>
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<tr>
<td>(m*,0,1/2)'</td>
<td>(6*,0,1/2)'</td>
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<td>Element</td>
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<td>(187.7.1445) P(2c) &amp; m'2 P(\delta c2)</td>
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<td>(188.1.1446) P(\delta c2)</td>
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<td>(188.2.1447) P(\delta c21')</td>
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<td>(188.3.1448) P(\delta c2)</td>
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<td>(188.4.1449) P(\delta c2)</td>
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<td>(188.5.1450) P(\delta c2)</td>
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<td>(189.1.1451) P(\delta 2m)</td>
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**MAGNETIC SPACE GROUP ELEMENTS** 140
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<th>Magnetic Space Group</th>
<th>Elements</th>
<th>Description</th>
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<td>189.2.1452 P6\textsuperscript{2}m\textsuperscript{1}</td>
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<td>189.3.1453 P6\textsuperscript{2}m P3\textsuperscript{1}m</td>
<td>(0,0,0; a,b,c)</td>
<td>(1\textsuperscript{<em>}0,0,0) (3\textsuperscript{</em>}0,0,0) (3\textsuperscript{-1}*0,0,0)</td>
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<td>(m\textsubscript{z}0,0,0) (\delta\textsubscript{z}0,0,0) (\delta\textsubscript{z}^{-1}*0,0,0)</td>
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<td>(2\textsuperscript{*}0,0,0) (2\textsubscript{xy}<em>0,0,0) (2\textsuperscript{</em>}0,0,0)</td>
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<td>(m\textsubscript{1}0,0,0) (m\textsubscript{2}0,0,0) (m\textsubscript{3}0,0,0)</td>
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<td>(m\textsubscript{z}0,0,0) (\delta\textsubscript{z}0,0,0) (\delta\textsubscript{z}^{-1}*0,0,0)</td>
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<td>(2\textsuperscript{*}0,0,0) (2\textsubscript{xy}<em>0,0,0) (2\textsuperscript{</em>}0,0,0)</td>
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<td>(mz *0,0,1/2)'</td>
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<td>(2<em>0,0,0) (6</em>0,0,0) (6*-1*0,0,0)</td>
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<td>191.4.1466 P6'/mm'm</td>
<td>P&amp;2m (0,0,0;a,b,c)</td>
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<td>191.5.1467 P6'/mmm</td>
<td>P&amp;m2 (0,0,0;a,b,c)</td>
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<td>P₆/mcc</td>
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<td>$(2_z*0,0,0)$</td>
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<td>$(2_z*0,0,1/2)$</td>
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<td>$(2_z*0,0,1/2)$</td>
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<td>$(6_z*0,0,0)$</td>
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<td>$(6_z*0,0,0)$</td>
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193.1.1485 P6\textsubscript{3}/mcm

\begin{align*}
&(1 \ast 0,0,0)' \\
&(m_z \ast 0,0,0)' \\
&(m_x \ast 0,1/2)' \\
&(m_1 \ast 0,0,0)'
\end{align*}

193.2.1486 P6\textsubscript{3}/mcm1'

\begin{align*}
&(1 \ast 0,0,0) \\
&(2_z \ast 0,0,1/2) \\
&(2_x \ast 0,0,1/2) \\
&(2_1 \ast 0,0,0) \\
&(m_z \ast 0,0,1/2) \\
&(m_x \ast 0,0,1/2) \\
&(m_1 \ast 0,0,0)
\end{align*}

193.3.1487 P6\textsubscript{3}/m'cm P6\textsubscript{3}cm

\begin{align*}
&(0,0,0; a,b,c) \\
&(1 \ast 0,0,0) \\
&(2_z \ast 0,0,1/2) \\
&(2_x \ast 0,0,1/2)' \\
&(2_1 \ast 0,0,0)' \\
&(m_z \ast 0,0,1/2)' \\
&(m_x \ast 0,0,1/2) \\
&(m_1 \ast 0,0,0) \\
&(3_z \ast 0,0,0) \\
&(6_z \ast 0,0,1/2) \\
&(2_{xy} \ast 0,0,1/2)' \\
&(2_2 \ast 0,0,0)' \\
&(m_{xy} \ast 0,0,1/2)' \\
&(m_2 \ast 0,0,0)' \\
&(3_{-1} \ast 0,0,0) \\
&(6_{-1} \ast 0,0,1/2) \\
&(2_{-1} \ast 0,0,1/2)' \\
&(2 \ast 0,0,0)' \\
&(m_{-1} \ast 0,0,1/2)' \\
&(m_{xy} \ast 0,0,1/2) \\
&(m_3 \ast 0,0,0)
\end{align*}

193.4.1488 P6\textsubscript{3}/mc'm P6\textsubscript{3}2m

\begin{align*}
&(0,0,1/4; a,b,c) \\
&(1 \ast 0,0,0) \\
&(2_z \ast 0,0,1/2) \\
&(2_x \ast 0,0,1/2) \\
&(2_1 \ast 0,0,0) \\
&(m_z \ast 0,0,1/2) \\
&(m_x \ast 0,0,1/2) \\
&(3_z \ast 0,0,0) \\
&(6_z \ast 0,0,1/2) \\
&(2_{xy} \ast 0,0,1/2) \\
&(2_2 \ast 0,0,0) \\
&(m_{xy} \ast 0,0,1/2) \\
&(3_{-1} \ast 0,0,0) \\
&(6_{-1} \ast 0,0,1/2) \\
&(2_{-1} \ast 0,0,1/2) \\
&(2 \ast 0,0,0) \\
&(m_{-1} \ast 0,0,1/2) \\
&(m_{xy} \ast 0,0,1/2) \\
&(m_3 \ast 0,0,0)
\end{align*}
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<th>P6c2</th>
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<th>(m₁*,0,0,0)</th>
<th>(m₂*,0,0,0)</th>
<th>(m₃*,0,0,0)</th>
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<td></td>
<td></td>
<td>(1*0,0,0)</td>
<td>(3*0,0,0)</td>
<td>(3⁻¹*0,0,0)</td>
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<td></td>
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<td></td>
<td>(2*0,0,1/2)²</td>
<td>(6*0,0,1/2)²</td>
<td>(6⁻¹*0,0,1/2)²</td>
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<td>(2x*0,0,1/2)²</td>
<td>(2y*0,0,1/2)²</td>
<td>(2*0,0,1/2)²</td>
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<td>(2*0,0,0)</td>
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<td>(δ*0,0,0)²</td>
<td>(δ*0,0,0)²</td>
<td>(δ⁻¹*0,0,0)²</td>
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<td>(m₂*0,0,1/2)²</td>
<td>(δ*0,0,1/2)²</td>
<td>(δ⁻¹*0,0,1/2)²</td>
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<td>(m₂*,0,0,0)²</td>
<td>(m₃*,0,0,0)²</td>
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<td>(1*0,0,0)</td>
<td>(3*0,0,0)</td>
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### CUBIC SYSTEM

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**Notes:**
- The superscript * indicates a magnetic field direction.
- The primes (') denote a magnetic field direction perpendicular to the crystallographic axes.
- The elements include translations, rotations, and screw axes.

**Magnetic Space Group Elements 152**
196.1.1506  F23  
(1*0,0,0)  (2*0,0,0)  (2*0,0,0)  (2*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
196.2.1507  F231'  
197.1.1508  I23  
(1*0,0,0)  (2*0,0,0)  (2*0,0,0)  (2*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
197.2.1509  I231'  
197.3.1510  I_p23  P23  (0,0,0;a,b,c)  
(1*0,0,0)  (2*0,0,0)  (2*0,0,0)  (2*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
198.1.1511  P2_3  
(1*0,0,0)  (2*1/2,1/2,0)  (2*0,1/2,1/2)  (2*1/2,0,1/2)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
198.2.1512  P2_31'  
199.1.1513  I2_3  
(1*0,0,0)  (2*1/2,1/2,0)  (2*0,1/2,1/2)  (2*1/2,0,1/2)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
(3*0,0,0)  (3*0,0,0)  (3*0,0,0)  (3*0,0,0)  
199.2.1514  I2_31'  

MAGNETIC SPACE GROUP ELEMENTS 153
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| 201.2.1521 | Pn\&l' |

| 201.3.1522 | Pn'\&' | P23 | (0,0,0;a,b,c) |
| (1\*0,0,0) | (2\*0,0,0) | (2\*0,0,0) | (2\*0,0,0) |
| (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) |
| (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) |
| (\&\*1/2,1/2,1/2)' | (m\*1/2,1/2,1/2)' | (m\*1/2,1/2,1/2)' | (m\*1/2,1/2,1/2)' |
| (\&\*1/2,1/2,1/2)' | (\&\*1/2,1/2,1/2)' | (\&\*1/2,1/2,1/2)' | (\&\*1/2,1/2,1/2)' |
| (\&\*1/2,1/2,1/2)' | (\&\*1/2,1/2,1/2)' | (\&\*1/2,1/2,1/2)' | (\&\*1/2,1/2,1/2)' |

| 201.4.1523 | P\&n\& | Fd\& | (0,0,0;2a,2b,2c) |
| (1\*0,0,0) | (2\*0,0,0) | (2\*0,0,0) | (2\*0,0,0) |
| (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) |
| (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) |
| (\&\*1/2,1/2,1/2) | (m\*1/2,1/2,1/2) | (m\*1/2,1/2,1/2) | (m\*1/2,1/2,1/2) |
| (\&\*1/2,1/2,1/2) | (\&\*1/2,1/2,1/2) | (\&\*1/2,1/2,1/2) | (\&\*1/2,1/2,1/2) |
| (\&\*1/2,1/2,1/2) | (\&\*1/2,1/2,1/2) | (\&\*1/2,1/2,1/2) | (\&\*1/2,1/2,1/2) |

| 202.1.1524 | Fm\&k |

| (1\*0,0,0) | (2\*0,0,0) | (2\*0,0,0) | (2\*0,0,0) |
| (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) |
| (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) | (3\*0,0,0) |
| (\&\*0,0,0) | (m\*0,0,0) | (m\*0,0,0) | (m\*0,0,0) |
| (\&\*0,0,0) | (\&\*0,0,0) | (\&\*0,0,0) | (\&\*0,0,0) |
| (\&\*0,0,0) | (\&\*0,0,0) | (\&\*0,0,0) | (\&\*0,0,0) |

MAGNETIC SPACE GROUP ELEMENTS 155
MAGNETIC SPACE GROUP ELEMENTS

202.2.1525 Fm\&1'

202.3.1526 Fm'\&' F23 (0,0,0;a,b,c)

203.1.1527 Fd&

203.2.1528 Fd&1'

203.3.1529 Fd'&' F23 (0,0,0;a,b,c)

204.1.1530 Im&
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**Magnetic Space Group Elements 157**
205.2.1536  Pa\&1'

205.3.1537  Pa'\&'  P2_13  (0,0,0; a,b,c)
(1*0,0,0)  (2_x*1/2,1/2,0)  (2_y*0,1/2,1/2)  (2_z*1/2,0,1/2)
(3_{xyz}*0,0,0)  (3_{xyz}^{-1}*0,0,0)  (3_{xyz}*0,1/2,1/2)  (3_{xyz}^{-1}*1/2,0,1/2)
(3_{xyz}*1/2,0,1/2)  (3_{xyz}^{-1}*1/2,1/2,0)  (3_{xyz}*1/2,1/2,0)  (3_{xyz}^{-1}*0,1/2,1/2)
(\&*0,0,0)'  (m_x*1/2,1/2,0)'  (m_y*0,1/2,1/2)'  (m_z*1/2,0,1/2)'
(\&_{xyz}*0,0,0)'  (\&_{xyz}^{-1}*0,0,0)'  (\&_{xyz}*0,1/2,1/2)'  (\&_{xyz}^{-1}*1/2,0,1/2)'
(\&_{xyz}^{-1}*1/2,1/2,0)'  (\&_{xyz}^{-1}*1/2,1/2,0)'

206.1.1538  Ia\&
(1*0,0,0)  (2_x*1/2,1/2,0)  (2_y*0,1/2,1/2)  (2_z*1/2,0,1/2)
(3_{xyz}*0,0,0)  (3_{xyz}^{-1}*0,0,0)  (3_{xyz}*0,1/2,1/2)  (3_{xyz}^{-1}*1/2,0,1/2)
(3_{xyz}^{-1}*1/2,1/2,0)  (3_{xyz}^{-1}*1/2,1/2,0)  (3_{xyz}*1/2,1/2,0)  (3_{xyz}*1/2,1/2,0)
(\&*0,0,0)  (m_x*1/2,1/2,0)  (m_y*0,1/2,1/2)  (m_z*1/2,0,1/2)
(\&_{xyz}*0,0,0)  (\&_{xyz}^{-1}*0,0,0)  (\&_{xyz}*0,1/2,1/2)  (\&_{xyz}^{-1}*1/2,0,1/2)
(\&_{xyz}^{-1}*1/2,1/2,0)  (\&_{xyz}^{-1}*1/2,1/2,0)

206.2.1539  Ia\&1'

206.3.1540  Ia'\&'  I2_3  (0,0,0; a,b,c)
(1*0,0,0)  (2_x*1/2,1/2,0)  (2_y*0,1/2,1/2)  (2_z*1/2,0,1/2)
(3_{xyz}*0,0,0)  (3_{xyz}^{-1}*0,0,0)  (3_{xyz}*0,1/2,1/2)  (3_{xyz}^{-1}*1/2,0,1/2)
(3_{xyz}^{-1}*1/2,1/2,0)  (3_{xyz}^{-1}*1/2,1/2,0)  (3_{xyz}*1/2,1/2,0)  (3_{xyz}*1/2,1/2,0)
(\&*0,0,0)'  (m_x*1/2,1/2,0)'  (m_y*0,1/2,1/2)'  (m_z*1/2,0,1/2)'
(\&_{xyz}*0,0,0)'  (\&_{xyz}^{-1}*0,0,0)'  (\&_{xyz}*0,1/2,1/2)'  (\&_{xyz}^{-1}*1/2,0,1/2)'
(\&_{xyz}^{-1}*1/2,1/2,0)'  (\&_{xyz}^{-1}*1/2,1/2,0)'

206.4.1541  I_p a\&  Pa\&  (0,0,0; a,b,c)
(1*0,0,0)  (2_x*1/2,1/2,0)  (2_y*0,1/2,1/2)  (2_z*1/2,0,1/2)
(3_{xyz}*0,0,0)  (3_{xyz}^{-1}*0,0,0)  (3_{xyz}*0,1/2,1/2)  (3_{xyz}^{-1}*1/2,0,1/2)
(3_{xyz}^{-1}*1/2,1/2,0)  (3_{xyz}^{-1}*1/2,1/2,0)  (3_{xyz}*1/2,1/2,0)  (3_{xyz}*1/2,1/2,0)
(\&*0,0,0)  (m_x*1/2,1/2,0)  (m_y*0,1/2,1/2)  (m_z*1/2,0,1/2)
(\&_{xyz}*0,0,0)  (\&_{xyz}^{-1}*0,0,0)  (\&_{xyz}*0,1/2,1/2)  (\&_{xyz}^{-1}*1/2,0,1/2)
(\&_{xyz}^{-1}*1/2,1/2,0)  (\&_{xyz}^{-1}*1/2,1/2,0)
| 207.1.1542 | P432 |
| (1*0,0,0) | (2*0,0,0) | (2*0,0,0) | (2*0,0,0) |
| (3*0,0,0) | (3*0,0,0) | (3*0,0,0) | (3*0,0,0) |
| (3*0,0,0) | (3*0,0,0) | (3*0,0,0) | (3*0,0,0) |
| (4*0,0,0) | (4*0,0,0) | (4*0,0,0) | (4*0,0,0) |
| 207.2.1543 | P4321' |

| 207.3.1544 | P4'32' P23 |
| (1*0,0,0) | (2*0,0,0) | (2*0,0,0) | (2*0,0,0) |
| (3*0,0,0) | (3*0,0,0) | (3*0,0,0) | (3*0,0,0) |
| (3*0,0,0) | (3*0,0,0) | (3*0,0,0) | (3*0,0,0) |
| (4*0,0,0) | (4*0,0,0) | (4*0,0,0) | (4*0,0,0) |
| 207.4.1545 | P4132 F432 |
| (1*0,0,0) | (2*0,0,0) | (2*0,0,0) | (2*0,0,0) |
| (3*0,0,0) | (3*0,0,0) | (3*0,0,0) | (3*0,0,0) |
| (3*0,0,0) | (3*0,0,0) | (3*0,0,0) | (3*0,0,0) |
| (4*0,0,0) | (4*0,0,0) | (4*0,0,0) | (4*0,0,0) |

MAGNETIC SPACE GROUP ELEMENTS 159
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<td>(3$_{xyz}$*0,0,0)</td>
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<td>(4$_x$*1/2,1/2,1/2)</td>
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<td>(4$_y$*1/2,1/2,1/2)</td>
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<td>(4$_y$*1/2,1/2,1/2)</td>
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<td>P$_F$4$_2$32</td>
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<td>(0,0,0;2a,2b,2c)</td>
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<td>209.2.1551</td>
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MAGNETIC SPACE GROUP ELEMENTS 160
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<td>(3*xyz,0,0) (3*xyz^{-1},0,0) (3*xyz,0,0) (3*xyz^{-1},0,0)</td>
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<tr>
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<td>(3*xyz*z,0,0) (3*xyz*z^{-1},0,0) (3*xyz*z,0,0) (3*xyz*z^{-1},0,0)</td>
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<tr>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<tr>
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<td>(3*xyz*z,0,0) (3*xyz*z^{-1},0,0) (3*xyz*z,0,0) (3*xyz*z^{-1},0,0)</td>
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<tr>
<td></td>
<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<tr>
<td>F4,321'</td>
<td>(1*0,0,0) (2*0,1/2,0,1/2) (2*0,1/2,1/2,0) (2*0,0,1/2,1/2)</td>
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<td>(3*xyz,0,0) (3*xyz^{-1},0,0) (3*xyz,0,0) (3*xyz^{-1},0,0)</td>
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<td>(3*xyz*z,0,0) (3*xyz*z^{-1},0,0) (3*xyz*z,0,0) (3*xyz*z^{-1},0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(3*xyz,0,0) (3*xyz^{-1},0,0) (3*xyz,0,0) (3*xyz^{-1},0,0)</td>
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<tr>
<td></td>
<td>(3*xyz*z,0,0) (3*xyz*z^{-1},0,0) (3*xyz*z,0,0) (3*xyz*z^{-1},0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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<td>(4*0,0,0) (4*0,0,0) (2*0,0,0) (2*0,0,0)</td>
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</table>
211.2.1557 I4321'  
(4z*0,0,0)  (4z*-1*0,0,0)  (2yz*0,0,0)  (2xz*0,0,0)

211.3.1558 I4'32'  I23 (0,0,0;a,b,c)  (1*0,0,0)  (2x*0,0,0)  (2y*0,0,0)  (2z*0,0,0)
(3xyz*0,0,0)  (3xyz*-1*0,0,0)  (3yz*0,0,0)  (3yz*-1*0,0,0)
(3xxy*0,0,0)  (3xxy*-1*0,0,0)  (3yzz*0,0,0)  (3yzz*-1*0,0,0)
(4x*0,0,0)'  (4x*-1*0,0,0)'  (2xyz*0,0,0)'  (2xyz*-1*0,0,0)'
(4y*0,0,0)'  (4y*-1*0,0,0)'  (2yzz*0,0,0)'  (2yzz*-1*0,0,0)'

211.4.1559 I 432  P432 (0,0,0;a,b,c)  (1*0,0,0)  (2x*0,0,0)  (2y*0,0,0)  (2z*0,0,0)
(3xyz*0,0,0)  (3xyz*-1*0,0,0)  (3yz*0,0,0)  (3yz*-1*0,0,0)
(3xxy*0,0,0)  (3xxy*-1*0,0,0)  (3yzz*0,0,0)  (3yzz*-1*0,0,0)
(4x*0,0,0)'  (4x*-1*0,0,0)'  (2xyz*0,0,0)'  (2xyz*-1*0,0,0)'
(4y*0,0,0)'  (4y*-1*0,0,0)'  (2yzz*0,0,0)'  (2yzz*-1*0,0,0)'

211.5.1560 Ip 432  P42 32 (0,0,0;a,b,c)  (1*0,0,0)  (2x*0,0,0)  (2y*0,0,0)  (2z*0,0,0)
(3xyz*0,0,0)  (3xyz*-1*0,0,0)  (3yz*0,0,0)  (3yz*-1*0,0,0)
(3xxy*0,0,0)  (3xxy*-1*0,0,0)  (3yzz*0,0,0)  (3yzz*-1*0,0,0)
(4x*1/2,1/2,1/2)  (4x*-1*1/2,1/2,1/2)  (2xyz*1/2,1/2,1/2)  (2xyz*-1*1/2,1/2,1/2)
(4y*1/2,1/2,1/2)  (4y*-1*1/2,1/2,1/2)  (2yz*1/2,1/2,1/2)  (2yz*-1*1/2,1/2,1/2)
(4z*1/2,1/2,1/2)  (4z*-1*1/2,1/2,1/2)  (2yzz*1/2,1/2,1/2)  (2yzz*-1*1/2,1/2,1/2)

212.1.1561 P4 3 32  
(1*0,0,0)  (2x*1/2,1/2,0)  (2y*0,1/2,1/2)  (2z*1/2,0,1/2)
(3xyz*0,0,0)  (3xyz*-1*0,0,0)  (3yz*0,1/2,1/2)  (3yz*-1*0,1/2,1/2)
(3xxy*1/2,0,1/2)  (3xxy*-1*1/2,0,1/2)  (3yzz*0,1/2,1/2)  (3yzz*-1*0,1/2,1/2)
### 212.2.1562 \(P4_3 32'\)

\[
\begin{align*}
\text{(1)*0,0,0} & \quad \text{(2)*1/2,1/2,0} & \quad \text{(2)*1/2,1/2,0} \\
(3xy)*0,0,0 & \quad (3xy)*1/2,0,0 & \quad (3xy)*0,1/2,1/2 \\
(3yz)*1/2,0,1/2 & \quad (3yz)*1/2,1/2,0 & \quad (3yz)*1/2,0,1/2 \\
(4x)*3/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 \\
(4y)*3/4,1/4,1/4 & \quad (4y)*1/4,1/4,3/4 & \quad (4y)*1/4,1/4,3/4 \\
(4z)*3/4,1/4,1/4 & \quad (4z)*1/4,3/4,1/4 & \quad (4z)*1/4,3/4,1/4 \\
\end{align*}
\]

### 212.3.1563 \(P4_3 32'\) \(P2_1 3\) \((0,0,0;a,b,c)\)

\[
\begin{align*}
\text{(1)*0,0,0} & \quad \text{(2)*1/2,1/2,0} & \quad \text{(2)*0,1/2,1/2} \\
(3xy)*0,0,0 & \quad (3xy)*1/2,0,0 & \quad (3xy)*0,1/2,1/2 \\
(3yz)*1/2,0,1/2 & \quad (3yz)*1/2,1/2,0 & \quad (3yz)*1/2,0,1/2 \\
(4x)*3/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 \\
(4y)*3/4,1/4,1/4 & \quad (4y)*1/4,1/4,3/4 & \quad (4y)*1/4,1/4,3/4 \\
(4z)*3/4,1/4,1/4 & \quad (4z)*1/4,3/4,1/4 & \quad (4z)*1/4,3/4,1/4 \\
\end{align*}
\]

### 213.1.1564 \(P4_1 32\)

\[
\begin{align*}
\text{(1)*0,0,0} & \quad \text{(2x)*1/2,1/2,0} & \quad \text{(2y)*1/2,1/2,0} \\
(3xy)*0,0,0 & \quad (3xy)*1/2,0,0 & \quad (3xy)*0,1/2,1/2 \\
(3yz)*1/2,0,1/2 & \quad (3yz)*1/2,1/2,0 & \quad (3yz)*1/2,0,1/2 \\
(4x)*3/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 \\
(4y)*3/4,1/4,1/4 & \quad (4y)*1/4,1/4,3/4 & \quad (4y)*1/4,1/4,3/4 \\
(4z)*3/4,1/4,1/4 & \quad (4z)*1/4,3/4,1/4 & \quad (4z)*1/4,3/4,1/4 \\
\end{align*}
\]

### 213.2.1565 \(P4_1 32'\)

\[
\begin{align*}
\text{(1)*0,0,0} & \quad \text{(2x)*1/2,1/2,0} & \quad \text{(2y)*1/2,1/2,0} \\
(3xy)*0,0,0 & \quad (3xy)*1/2,0,0 & \quad (3xy)*0,1/2,1/2 \\
(3yz)*1/2,0,1/2 & \quad (3yz)*1/2,1/2,0 & \quad (3yz)*1/2,0,1/2 \\
(4x)*3/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 \\
(4y)*3/4,1/4,1/4 & \quad (4y)*1/4,1/4,3/4 & \quad (4y)*1/4,1/4,3/4 \\
(4z)*3/4,1/4,1/4 & \quad (4z)*1/4,3/4,1/4 & \quad (4z)*1/4,3/4,1/4 \\
\end{align*}
\]

### 213.3.1566 \(P4_1 32'\) \(P2_1 3\) \((0,0,0;a,b,c)\)

\[
\begin{align*}
\text{(1)*0,0,0} & \quad \text{(2x)*1/2,1/2,0} & \quad \text{(2y)*1/2,1/2,0} \\
(3xy)*0,0,0 & \quad (3xy)*1/2,0,0 & \quad (3xy)*0,1/2,1/2 \\
(3yz)*1/2,0,1/2 & \quad (3yz)*1/2,1/2,0 & \quad (3yz)*1/2,0,1/2 \\
(4x)*3/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 & \quad (4x)*1/4,3/4,3/4 \\
(4y)*3/4,1/4,1/4 & \quad (4y)*1/4,1/4,3/4 & \quad (4y)*1/4,1/4,3/4 \\
(4z)*3/4,1/4,1/4 & \quad (4z)*1/4,3/4,1/4 & \quad (4z)*1/4,3/4,1/4 \\
\end{align*}
\]

### 214.1.1567 \(I4_3 2\)

\[
\begin{align*}
\text{(1)*0,0,0} & \quad \text{(2x)*1/2,1/2,0} & \quad \text{(2y)*1/2,1/2,0} \\
(3xy)*0,0,0 & \quad (3xy)*1/2,0,0 & \quad (3xy)*0,1/2,1/2 \\
(3yz)*1/2,0,1/2 & \quad (3yz)*1/2,1/2,0 & \quad (3yz)*1/2,0,1/2 \\
(4x)*3/4,1/4,3/4 & \quad (4x)*1/4,3/4,1/4 & \quad (4x)*1/4,3/4,1/4 \\
(4y)*3/4,1/4,1/4 & \quad (4y)*1/4,1/4,3/4 & \quad (4y)*1/4,1/4,3/4 \\
(4z)*3/4,1/4,1/4 & \quad (4z)*1/4,3/4,1/4 & \quad (4z)*1/4,3/4,1/4 \\
\end{align*}
\]
214.2.1568  I4,321'  

(4y 3/4,1/4,1/4)  
(4z 1/4,3/4,1/4)  
(2xz 1/4,1/4,3/4)  
(2g 3/4,3/4,3/4) 

(4y -1/4,1/4,3/4)  
(4z -1/4,1/4,1/4)  
(2yz 1/4,3/4,1/4)  
(2g -1/4,3/4,3/4) 

214.3.1569  I4 132'  

(0,0,0;a,b,c)  
(1*0,0,0)  
(2*0,1/2,1/2)  
(2*1/2,0,1/2) 

(3*1/2,1/2,0)  
(3*0,1/2,1/2)  
(3*0,1/2,1/2)  
(3*1/2,1/2,0) 

(4x 1/4,1/4,3/4)  
(4x -1/2,1/2,2,0)  
(2x 3/4,1/4,1/4)  
(2x -1/4,1/4,3/4) 

(4y 1/4,3/4,1/4)  
(4y 1/4,3/4,1/4)  
(2y 1/4,3/4,1/4)  
(2y 1/4,3/4,1/4) 

(4z 1/4,3/4,1/4)  
(4z 1/4,3/4,1/4)  
(2z 1/4,3/4,1/4)  
(2z 1/4,3/4,1/4) 

214.4.1570  I 4132  

(0,0,0;a,b,c)  
(1*0,0,0)  
(2*0,1/2,1/2)  
(2*1/2,0,1/2) 

(3*1/2,1/2,0)  
(3*0,1/2,1/2)  
(3*0,1/2,1/2)  
(3*1/2,1/2,0) 

(4x 1/4,1/4,3/4)  
(4x 1/4,1/4,1/4)  
(2x 3/4,1/4,1/4)  
(2x 1/4,3/4,3/4) 

(4y 1/4,1/4,3/4)  
(4y 1/4,1/4,1/4)  
(2y 1/4,1/4,3/4)  
(2y 1/4,1/4,3/4) 

(4z 1/4,3/4,1/4)  
(4z 1/4,1/4,3/4)  
(2z 1/4,3/4,1/4)  
(2z 1/4,3/4,1/4) 

214.5.1571  I 4132'  

(0,0,0;a,b,c)  
(1*0,0,0)  
(2*0,1/2,1/2)  
(2*1/2,0,1/2) 

(3*1/2,1/2,0)  
(3*0,1/2,1/2)  
(3*0,1/2,1/2)  
(3*1/2,1/2,0) 

(4x 1/4,3/4,3/4)  
(4x 1/4,3/4,1/4)  
(2x 3/4,1/4,3/4)  
(2x 1/4,3/4,3/4) 

(4y 1/4,3/4,3/4)  
(4y 1/4,3/4,1/4)  
(2y 3/4,1/4,3/4)  
(2y 1/4,3/4,3/4) 

(4z 1/4,3/4,3/4)  
(4z 1/4,3/4,1/4)  
(2z 3/4,1/4,3/4)  
(2z 1/4,3/4,3/4) 

215.1.1572  P 43m  

(1*0,0,0)  
(2*0,0,0)  
(2*0,0,0)  
(2*0,0,0) 

(3*0,0,0)  
(3*0,0,0)  
(3*0,0,0)  
(3*0,0,0) 

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(3*0,0,0)  
(3*0,0,0) 

215.2.1573  P 43m1'
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| F & 3m1' | | | | |

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<td>$(2_y*0,0,0)$</td>
<td>$(2_z*0,0,0)$</td>
<td>$(1*0,0,0)$</td>
<td>$(2_x*0,0,0)$</td>
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<td>$(4_y*0,0,0)$</td>
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<td>$(5_y*0,0,0)'$</td>
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MAGNETIC SPACE GROUP ELEMENTS 166
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<th>218.2.1586 P43n1'</th>
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<td>(4x1/2,1/2,1/2) (4y1/2,1/2,1/2) (4z1/2,1/2,1/2) (m_{xz}^*1/2,1/2,1/2) (m_{yz}^*1/2,1/2,1/2)</td>
<td>(10,0,0) (2_{x}^*0,0,0) (2_{y}^*0,0,0) (2_{z}^*0,0,0) (2_{x}^*0,0,0)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
<td>(10,0,0) (2_{x}^*0,0,0) (2_{y}^*0,0,0) (2_{z}^*0,0,0) (2_{x}^*0,0,0)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
</tr>
<tr>
<td>(4x1/2,1/2,1/2) (4y1/2,1/2,1/2) (4z1/2,1/2,1/2) (m_{xz}^*1/2,1/2,1/2) (m_{yz}^*1/2,1/2,1/2)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
<td>(10,0,0) (2_{x}^*0,0,0) (2_{y}^*0,0,0) (2_{z}^*0,0,0) (2_{x}^*0,0,0)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
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<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
<td>(3_{xyz}^*0,0,0) (3_{xyz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0) (3_{x&amp; yz}^{-1}*0,0,0) (3_{x&amp; yz}^*0,0,0)</td>
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<td>(10,0,0) (2_{x}^*0,0,0) (2_{y}^*0,0,0) (2_{z}^*0,0,0) (2_{x}^*0,0,0)</td>
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MAGNETIC SPACE GROUP ELEMENTS 167
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221.2.1595  Pm\&m 1'

221.3.1596  Pm'&m   P&3m  (0,0,0;a,b,c)

221.4.1597  Pm&m'   Pm&   (0,0,0;a,b,c)

221.5.1598  Pm'&m'   P432   (0,0,0;a,b,c)

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MAGNETIC SPACE GROUP ELEMENTS 169
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MAGNETIC SPACE GROUP ELEMENTS 172
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MAGNETIC SPACE GROUP ELEMENTS 173
MAGNETIC SPACE GROUP ELEMENTS

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(4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)
(4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)

224.1.1611  Pn&m

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(3,x*yz*0,0)  (3,x*yz*0,0)  (3,x*yz*0,0)  (3,x*yz*0,0)
(4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)
(4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)

224.2.1612  Pn&m1

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(3,x*yz*0,0)  (3,x*yz*0,0)  (3,x*yz*0,0)  (3,x*yz*0,0)
(4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)
(4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)  (4,xyz*1/2,1/2,1/2)

MAGNETIC SPACE GROUP ELEMENTS 174
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MAGNETIC SPACE GROUP ELEMENTS 180
227.4.1631  Fd&m'  Fd&  (0,0,0; a,b,c)

227.5.1632  Fd&m'  F4,32  (0,0,0; a,b,c)
## MAGNETIC SPACE GROUP ELEMENTS

### 228.1633 Fd\&c

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<tr>
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### 228.4.1636 Fd\&c' Fd\&

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228.1.1638  Im&m

228.5.1637  Fd'ac' F4_32 (1/8,1/8,1/8;a,b,c)
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(3*0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0)
(3*0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0)
(3*0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0)
(4,1/2,1/2,1/2) (4,1/2,1/2,1/2) (4,1/2,1/2,1/2) (4,1/2,1/2,1/2) (4,1/2,1/2,1/2)
(4,1/2,1/2,1/2) (4,1/2,1/2,1/2) (4,1/2,1/2,1/2) (4,1/2,1/2,1/2) (4,1/2,1/2,1/2)

229.9.1646  l_p, m&m'  Pn&n  (0,0,0; a,b,c)
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(3*0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0)
(3*0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0)
(3*0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0) (3,0,0,0)
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230.1.1647  l&d
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(4,1/4,1,3/4) (4,1/4,1,3/4) (4,1/4,1,3/4) (4,1/4,1,3/4) (4,1/4,1,3/4)
(5 \times y^{3/4,1/4,1/4})' (5 \times y^{-1} * 1/4,1/4,1/4)' (m xz * 1/4,1/4,3/4)' (m x * 1/4,3/4,3/4)'

(5 \times z^{1/4,3/4,1/4})' (5 \times z^{-1} * 1/4,1/4,3/4)' (m yz * 1/4,3/4,1/4)' (m y * 3/4,3/4,3/4)'

(1 * 0,0,0)' (2 \times * 1/2,1/2,0)' (2 \times * 0,1/2,1/2)' (2 \times * 1/2,1/2,0)' (2 \times * 1/2,0,1/2)'

(3 \times y^{0,0,0})' (3 \times y^{-1} * 0,0,0)' (3 \times y^{0,1/2,1/2})' (3 \times y^{-1} * 1/2,0,1/2)'

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I4_32 (0,0,0; a, b, c)
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xy z

(100) (m, 00) (m, 00) (2, 00)

(00; a, b) (100) (m, 00)' (m, 00)' (2, 00)'

(00; a, b) (100) (m, 00) (m, 00)' (2, 00)'

(00; 2a, b) (100) (m, 00) (m, 00) (2, 00)

(00; 2a, b) (100) (m, 00) (m, 00) (2, 00)

(00; a, b) (100) (m, 00)' (m, 00)' (2, 00)'

(00; a, b) (100) (m, 00) (m, 00) (2, 00)

(00; a, (a+b)/2) (100) (m, 00)' (m, 00)' (2, 00)'

(00; a, (a+b)/2) (100) (m, 00) (m, 00)' (2, 00)'

(00; a, b) (100) (m, 00) (m, 00) (2, 00)

(00; a, b) (100) (m, 00)' (m, 00)' (2, 00)'

(¼¼; a, b) (100) (m, 00) (m, 00) (2, 00)
| 10.1.49 | p4 | (1|00) | (4z|00) | (2z|00) | (4z⁻¹|00) |
|---------|----|------|--------|--------|---------|
| 10.2.50 | p41' |      |        |        |         |
| 10.3.51 | p4' | p211 | (00;a,b) | (1|00) | (4z|00)' | (2z|00) | (4z⁻¹|00)'
| 10.4.52 | p₄⁴ | p4 | (00;a-b,a+b) | (1|00) | (4z|00) | (2z|00) | (4z⁻¹|00) |

| 11.1.53 | p4mm | (1|00) | (4z|00) | (2z|00) | (4z⁻¹|00) |
|---------|------|--------|--------|--------|---------|
|         |      | (mₓ|00) | (mᵧ|00) | (mₓᵧ|00) | (mₓᵧ|00) |
| 11.2.54 | p4mm1' |      |        |        |         |

| 11.3.55 | p4m'm' | p4 | (00;a,b) | (1|00) | (4z|00) | (2z|00) | (4z⁻¹|00) |
|         |       |      |         | (mₓ|00)' | (mᵧ|00)' | (mₓᵧ|00)' | (mₓᵧ|00)'
| 11.4.56 | p4'm'm' | p2mm | (00;a,b) | (1|00) | (4z|00)' | (2z|00) | (4z⁻¹|00)'
|         |       |      |         | (mₓ|00) | (mᵧ|00) | (mₓᵧ|00)' | (mₓᵧ|00)'
| 11.5.57 | p4'm'm' | c2mm | (00;a-b,a+b) | (1|00) | (4z|00)' | (2z|00) | (4z⁻¹|00)'
|         |       |      |         | (mₓ|00)' | (mᵧ|00)' | (mₓᵧ|00) | (mₓᵧ|00) |
| 11.6.58 | p₄⁴m'm' | p4gm | (00;a-b,a+b) | (1|00) | (4z|00) | (2z|00) | (4z⁻¹|00) |
|         |       |      |         | (mₓ|10) | (mᵧ|10) | (mₓᵧ|10) | (mₓᵧ|10) |
| 11.7.59 | p₄⁴mm | p4mm | (00;a-b,a+b) | (1|00) | (4z|00) | (2z|00) | (4z⁻¹|00) |
|         |       |      |         | (mₓ|00) | (mᵧ|00) | (mₓᵧ|00) | (mₓᵧ|00) |
| 12.1.60 | p4gm | (1|00) | (4z|00) | (2z|00) | (4z⁻¹|00) |
|         |       | (mₓ|½½) | (mᵧ|½½) | (mₓᵧ|½½) | (mₓᵧ|½½) |

MAGNETIC SPACE GROUP ELEMENTS 191
| 12.2.61 | p4gm1' |
| 12.3.62 | p4g'm' p4 (00;a,b) | (1|00) (4z|00) (2z|00) (4z\(^{-1}\)|00) |
|         |                  | (m\(_x\)|½½\(^\prime\)) (m\(_y\)|½½\(^\prime\)) (m\(_{xy}\)|½½\(^\prime\)) |
| 12.4.63 | p4'gm' p2gg (00;a,b) | (1|00) (4z|00\(^\prime\)) (2z|00) (4z\(^{-1}\)|00\(^\prime\)) |
|         |                  | (m\(_x\)|½½) (m\(_y\)|½½) (m\(_{xy}\)|½½\(^\prime\)) |
| 12.5.64 | p4'g'm c2mm (½0;a-b,a+b) | (1|00) (4z|00\(^\prime\)) (2z|00) (4z\(^{-1}\)|00\(^\prime\)) |
|         |                  | (m\(_x\)|½½\(^\prime\)) (m\(_y\)|½½\(^\prime\)) (m\(_{xy}\)|½½) |
| 13.1.65 | p3 | (1|00) (3z|00) (3z\(^{-1}\)|00) |
| 13.2.66 | p31' |
| 14.1.67 | p3m1 | (1|00) (3z|00) (3z\(^{-1}\)|00) |
|         |                  | (m\(_x\)|00) (m\(_y\)|00) (m\(_{xy}\)|00) |
| 14.2.68 | p3m11' |
| 14.3.69 | p3m'1 p3 (00;a,b) | (1|00) (3z|00) (3z\(^{-1}\)|00) |
|         |                  | (m\(_x\)|00\(^\prime\)) (m\(_y\)|00\(^\prime\)) (m\(_{xy}\)|00\(^\prime\)) |
| 15.1.70 | p31m | (1|00) (3z|00) (3z\(^{-1}\)|00) |
|         |                  | (m\(_l\)|00) (m\(_z\)|00) (m\(_z\)|00) |
| 15.2.71 | p31m1' |

MAGNETIC SPACE GROUP ELEMENTS 192
| 15.3.72 | p31m' | p3 | (00; a,b) | (1 | 00) | (3 | 00) | (3Z^-1 | 00) |
|         |       |    |           | (m1 | 00)' | (m2 | 00)' | (m3 | 00)' |
| 16.1.73 | p6   |    |           | (1 | 00) | (3 | 00) | (3Z^-1 | 00) |
|         |       |    |           | (6 | 00) | (2 | 00) | (6Z^-1 | 00) |
| 16.2.74 | p61' |    |           |      |      |        |
| 16.3.75 | p6'  | p3 | (00; a,b) | (1 | 00) | (3 | 00) | (3Z^-1 | 00) |
|         |       |    |           | (6 | 00) | (2 | 00) | (6Z^-1 | 00) |
| 17.1.76 | p6mm |    |           | (1 | 00) | (3 | 00) | (3Z^-1 | 00) |
|         |       |    |           | (6 | 00) | (2 | 00) | (6Z^-1 | 00) |
|         |       |    |           | (m | 00) | (m | 00) | (m | 00) |
| 17.2.77 | p6mm1' | |           |      |      |        |
| 17.3.78 | p6m'm' | p6 | (000; a,b) | (1 | 00) | (3 | 00) | (3Z^-1 | 00) |
|         |       |    |           | (6 | 00) | (2 | 00) | (6Z^-1 | 00) |
|         |       |    |           | (m | 00)' | (m | 00)' | (m | 00)' |
| 17.4.79 | p6'm'm' | p3m1 | (00; a,b) | (1 | 00) | (3 | 00) | (3Z^-1 | 00) |
| 17.5.80 | p6'm'm | p31m | (00; a, b) | (6z|00)' | (2z|00)' | (6z⁻¹|00)' |
|---------|--------|-------|-----------|----------|----------|----------|
|         |        |       |            | (m_x|00)   | (m_y|00)   | (m_y|00)   |
|         |        |       |            | (m_x|00)'  | (m_y|00)'  | (m_y|00)'  |
|         |        |       |            | (m_x|00)   | (m_y|00)   | (m_y|00)   |
|         |        |       |            | (m_x|00)'  | (m_y|00)'  | (m_y|00)'  |
|         |        |       |            | (m_x|00)   | (m_y|00)   | (m_y|00)   |
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<td>2.4.7</td>
<td>$p_{2a}m$</td>
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MAGNETIC SPACE GROUP ELEMENTS 195
<table>
<thead>
<tr>
<th>Crystal system</th>
<th>Restrictions on cell parameter</th>
<th>Parameters to be determined</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Triclinic</strong></td>
<td>None</td>
<td>a,b,c; α,β,γ</td>
</tr>
<tr>
<td><strong>Monoclinic</strong></td>
<td>α = γ = 90°</td>
<td>a,b,c; γ</td>
</tr>
<tr>
<td><strong>Orthorhombic</strong></td>
<td>α = β = γ = 90°</td>
<td>a,b,c</td>
</tr>
<tr>
<td><strong>Tetragonal</strong></td>
<td>a = b; α = β = γ = 90°</td>
<td>a,c</td>
</tr>
<tr>
<td><strong>Trigonal</strong></td>
<td>Hexagonal axes: a = b; α = β = γ = 90°</td>
<td>a,c</td>
</tr>
<tr>
<td><strong>Hexagonal</strong></td>
<td>a = b; α = β = γ = 120°</td>
<td>a,c</td>
</tr>
<tr>
<td><strong>Cubic</strong></td>
<td>a = b = c; α = β = γ = 90°</td>
<td>a</td>
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### Two-Dimensional

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<td>a,b,γ</td>
</tr>
<tr>
<td><strong>Rectangular</strong></td>
<td>γ = 90°</td>
<td>a,b</td>
</tr>
<tr>
<td><strong>Square</strong></td>
<td>a = b</td>
<td>a</td>
</tr>
<tr>
<td><strong>Hexagonal</strong></td>
<td>a = b; γ = 120°</td>
<td>a</td>
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### One Dimensional

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<tbody>
<tr>
<td><strong>----------</strong></td>
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<td>a</td>
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Table 1.3.1: Symmetry directions and position in Hermann-Mauguin symbols

Directions which belong to the same set of equivalent symmetry directions are given between braces. The first entry in each set is taken as the representative of that set.

**Three-Dimensional**

<table>
<thead>
<tr>
<th>Lattice</th>
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<th>Secondary</th>
<th>Tertiary</th>
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<td></td>
</tr>
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<td>[010]</td>
<td>unique axis b</td>
<td></td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>[100]</td>
<td>[010]</td>
<td>[001]</td>
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<tr>
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<td></td>
<td>{[100]}</td>
<td>{[1\overline{1}0]}</td>
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<tr>
<td>Hexagonal</td>
<td>[001]</td>
<td>{[100]}</td>
<td>{[1\overline{1}0]}</td>
</tr>
<tr>
<td>Hexagonal (hexagonal axes)</td>
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<tr>
<td>Rhombohedral</td>
<td>[001]</td>
<td>{[100]}</td>
<td>{[1\overline{1}0]}</td>
</tr>
<tr>
<td>Cubic</td>
<td>{[100]}</td>
<td>{[11\overline{1}]}</td>
<td>{[1\overline{1}0]}</td>
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<tr>
<td></td>
<td>{[010]}</td>
<td>{[1\overline{1}1]}</td>
<td>{[1\overline{1}]0}</td>
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<td></td>
<td>{[001]}</td>
<td>{[1\overline{1}]1}</td>
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Table 1.3.1 - 1
# Two-Dimensional

Symmetry direction  
(position in Hermann-Mauguin symbol)

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<th>Tertiary</th>
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<tr>
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<tr>
<td>Rectangular</td>
<td>Rotation Point in Plane</td>
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<td>[01]</td>
</tr>
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<td>Square</td>
<td>Rotation Point in Plane</td>
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<td>{[1 \bar{1}]}</td>
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<tr>
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<td>{[1 \bar{1}]}</td>
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<td></td>
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# Table 1.3.2: Symmetry direction subindex symbols

## Three-Dimensional

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<td>Orthorhomic</td>
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</tr>
<tr>
<td></td>
<td>[010]</td>
<td>y</td>
</tr>
<tr>
<td></td>
<td>[001]</td>
<td>z</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>[001]</td>
<td>z</td>
</tr>
<tr>
<td></td>
<td>[100]</td>
<td>x</td>
</tr>
<tr>
<td></td>
<td>[010]</td>
<td>y</td>
</tr>
<tr>
<td></td>
<td>[110]</td>
<td>xy</td>
</tr>
<tr>
<td></td>
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</tr>
<tr>
<td>Hexagonal</td>
<td>[001]</td>
<td>z</td>
</tr>
<tr>
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<td>[100]</td>
<td>x</td>
</tr>
<tr>
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<td>[010]</td>
<td>y</td>
</tr>
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</tr>
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<td>Cubic</td>
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<tr>
<td></td>
<td>[010]</td>
<td>y</td>
</tr>
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TABLE 1.3.2 - 1
## Two-dimensional

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<th>Lattice</th>
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<tr>
<td>Oblique</td>
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<tr>
<td></td>
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<td>x</td>
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<tr>
<td></td>
<td>[01]</td>
<td>y</td>
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<tr>
<td>Square</td>
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<td>x</td>
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<tr>
<td></td>
<td>[01]</td>
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<td>x</td>
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<td></td>
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![Oblique Diagram](image1.png)

![Rectangular Diagram](image2.png)

![Rectangular Diagram](image3.png)

![Hexagonal Diagram](image4.png)

**TABLE 1.3.2 - 2**
### Tables 1.4: Comparison of Magnetic Space Group and Black and White Space Group Symbols

#### Table 1.4 - 3D

**Three-dimensional:** Opechowski and Guccione (OG) symbols, Table 1.1-3D, compared with Belov, Neronova and Smirnova (BNS) symbols (1955, 1957). If the symbols are the same, no symbol is given in the BNS column.

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<th>BNS</th>
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<td>4.2.16</td>
<td>P2_1'</td>
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<tr>
<td>1.3.3 P_2s 1</td>
<td>P_1</td>
<td>4.3.17</td>
<td>P2_1'</td>
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<tr>
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<td>4.4.18</td>
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<td>P_a 2_1</td>
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<tr>
<td>2.2.5 P_11'</td>
<td>5.1.19</td>
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<td>2.3.6 P_1'</td>
<td>5.2.20</td>
<td>C2_1'</td>
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<td>2.4.7 P_2s_1</td>
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<table>
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<th></th>
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<td>5.5.23</td>
<td>C_p 2</td>
<td>P_c 2</td>
</tr>
<tr>
<td>3.2.9 P21'</td>
<td>5.6.24</td>
<td>C_p 2_1</td>
<td>P_c 2_1</td>
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<td>6.1.25</td>
<td>Pm</td>
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<tr>
<td>3.4.11 P_2a 2</td>
<td>P_a 2</td>
<td>6.2.26</td>
<td>Pm_1'</td>
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<tr>
<td>3.5.12 P_2b 2</td>
<td>P_b 2</td>
<td>6.3.27</td>
<td>Pm_1'</td>
</tr>
<tr>
<td>3.6.13 P_c 2</td>
<td>C_a 2</td>
<td>6.4.28</td>
<td>P_2a m</td>
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<td>3.7.14 P_2b 2'</td>
<td>P_b 2_1</td>
<td>6.5.29</td>
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*TABLE 1.4 - 3D - 1*
<p>| | | | | |</p>
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<td>10.3.51</td>
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<td>7.2.33</td>
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<td>P&lt;sub&gt;a&lt;/sub&gt;c</td>
<td>10.9.57</td>
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<td>7.5.36</td>
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<td>P&lt;sub&gt;b&lt;/sub&gt;c</td>
<td>10.10.58</td>
<td>P&lt;sub&gt;2c&lt;/sub&gt;2'/m</td>
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<tr>
<td>7.6.37</td>
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<td>C&lt;sub&gt;a&lt;/sub&gt;c</td>
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<td><strong>8.1.38</strong></td>
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<td>P2&lt;sub&gt;y&lt;/sub&gt;'/m</td>
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**TABLE 1.4 - 3D - 2**
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<td>2/m'</td>
<td>P2</td>
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| 39.11.288 | Aₚ bm'²' | Pₜ ca²₁ | 42.2.310 | Fmm21' |
| 39.12.289 | Aₚ b'm²' | Pₐ cc² | 42.3.311 | Fm'm²' |
| 39.13.290 | Aₙ b'm²' | lₙ ba2 | 42.4.312 | Fm'm²' |
| 40.1.291 | Ama2 | 42.5.313 | F₁ₙ mm² | Cₐ mm² |
| 40.2.292 | Ama21' | 42.6.314 | Fₐ mm² | Aₐ mm² |
| 40.3.293 | Am'a2' | 42.7.315 | F₁ₚ mm²' | Cₐ mc²₁ |
| 40.4.294 | Ama'2 | 42.8.316 | F₁ₚ m'm² | Cₐ cc² |
| 40.5.295 | Am'a2 | 42.9.317 | Fₐ m'm²' | Aₐ bm² |
| 40.6.296 | Aₚ ma2 | Pₐ ma2 | 42.10.318 | Fₐ mm²' | Aₐ ma2 |
| 40.7.297 | Aₚ m'a2' | Pₐ na₂₁ | 42.11.319 | Fₐ m'm² | Aₐ ba2 |
| 40.8.298 | Aₚ ma'2' | Pₐ mn²₁ | 43.1.320 | Fdd2 |
| 40.9.299 | Aₚ m'a2 | Pₐ nn² | 43.2.321 | Fdd21' |
| 41.1.300 | Aba2 | 43.3.322 | Fd'd²' |
| 41.2.301 | Aba21' | 43.4.323 | Fd'd² |
| 41.3.302 | Ab'a2' | 44.1.324 | Imm² |
| 41.4.303 | Ab'a2 | 44.2.325 | Imm21' |
| 41.5.304 | Ab'a2 | 44.3.326 | Im'm² |
| 41.6.305 | Aₚ ba2 | Pₐ ba2 | 44.4.327 | Im'm² |
| 41.7.306 | Aₚ b'a2' | Pₐ ca²₁ | 44.5.328 | Iₚ mm² | P₁ₚ mm² |
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| 107.8.890 | l_p, 4'm'm' | P, 4_2 mc | | |
| 107.9.891 | l_p, 4'm'm' | P, 4 mc | 111.1.911 | P42m |
| | | | 111.2.912 | P42m1' |
| 108.1.892 | l4cm | 111.3.913 | P4'2'm |
| 108.2.893 | l4cm1' | 111.4.914 | P4'2m' |
| 108.3.894 | l4'c'm | 111.5.915 | P42'm' |
| 108.4.895 | l4'cm' | 111.6.916 | P_2c 42m | P_c 42m |
| 108.5.896 | l4'cm' | 111.7.917 | P_p 42m | P_c 4m2 |
| 108.6.897 | l_p, 4cm | P, 4bm | 111.8.918 | P_1 42m | l_c 4m2 |
| 108.7.898 | l_p, 4'c'm | P, 4_2 cm | 111.9.919 | P_2c 42'm' | P_c 42c |
| 108.8.899 | l_p, 4'cm' | P, 4_2 bc | 111.10.920 | P_p 4'2m' | P_c 4b2 |
| 108.9.900 | l_p, 4c'm' | P, 4cc | 111.11.921 | P_1 4'2m' | l_c 4c2 |
| 109.1.901 | l4, md | 112.1.922 | P42c |
| 109.2.902 | l4, md1' | 112.2.923 | P42c1' |
| 109.3.903 | l4,'m'd | 112.3.924 | P4'2c' |
| 109.4.904 | l4,'md' | 112.4.925 | P4'2c' |
| 109.5.905 | l4,'m'd' | 112.5.926 | P42'c' |
| | | | 112.6.927 | P_p 42c | P_c 4c2 |
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| 135.7.1149 | P4 \textsubscript{2}/mb'c' | 138.1.1170 | P4 \textsubscript{2}/ncm |
| 135.8.1150 | P4 \textsubscript{2}/m'bc' | 138.2.1171 | P4 \textsubscript{2}/ncm1' |
| 135.9.1151 | P4 \textsubscript{2}/m'b'c' | 138.3.1172 | P4 \textsubscript{2}/n'c' |
| 136.1.1152 |  **P4 \textsubscript{2}/nmn** | 138.4.1173 | P4 \textsubscript{2}/nc'm |
| 136.2.1153 | P4 \textsubscript{2}/nmn1' | 138.5.1174 | P4 \textsubscript{2}/nc'm' |
| 136.3.1154 | P4 \textsubscript{2}/m'n'm | 138.6.1175 | P4 \textsubscript{2}/n'c'm |
| 136.4.1155 | P4 \textsubscript{2}/mn'm | 138.7.1176 | P4 \textsubscript{2}/nc'm' |
| 136.5.1156 | P4 \textsubscript{2}/mn'm' | 138.8.1177 | P4 \textsubscript{2}/n'c'm' |
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| 136.7.1158 | P4 \textsubscript{2}/mn'm' | 139.1.1179 | I4/mmm |
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| 136.9.1160 | P4 \textsubscript{2}/m'n'm' | 139.3.1181 | I4/m'mm |
| 137.1.1161 |  **P4 \textsubscript{2}/nmc** | 139.4.1182 | I4'/mm'm |
| 137.2.1162 | P4 \textsubscript{2}/nmc1' | 139.5.1183 | I4'/mmm' |
| 137.3.1163 | P4 \textsubscript{2}/n'mc | 139.6.1184 | I4'/m'm'm |
| 137.4.1164 | P4 \textsubscript{2}/nm'c | 139.7.1185 | I4/mm'm' |
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| 137.6.1166 | P4 \textsubscript{2}/n'mc | 139.9.1187 | I4/m'm'm' |
| 137.7.1167 | P4 \textsubscript{2}/nm'c' | 139.10.1188 | I_{p} 4/mmm |
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**TABLE 1.4 - 3D - 28**
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TABLE 1.4 - 3D - 29
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**160.1.1295** R₃m

| 155.2.1276 | R₃₂₁' | 160.2.1296 | R₃m₁' |
| 155.3.1277 | R₃₂' | 160.3.1297 | R₃m' |
| 155.4.1278 | R₉₃₂ | R₉₃₂ | 160.4.1298 | R₉₃m | R₉₃m |
|            |      |      | 160.5.1299 | R₉₃m' | R₉₃c |

**156.1.1279** P₃m₁  
| 161.1.1300 | R₃c |

| 156.2.1280 | P₃m₁₁' | 161.2.1301 | R₃c₁' |
| 156.3.1281 | P₃m₁' | 161.3.1302 | R₃c' |
| 156.4.1282 | P₂c₃m₁ | P₃m₁ | 161.4.1303 | P₃₁m |
| 156.5.1283 | P₂c₃m₁' | P₃c₁ |

**157.1.1284** P₃₁m  
| 162.1.1304 | P₃₁m₁' |

| 157.2.1285 | P₃₁m₁' | 162.3.1305 | P₃'₁m |
| 157.3.1286 | P₃₁m' | 162.4.1306 | P₃'₁m' |
| 157.4.1287 | P₂c₃₁m | P₃₁m | 162.5.1307 | P₃₁m' |
| 157.5.1288 | P₂c₃₁m' | P₃₁c | 162.6.1308 | P₂c₃₁m | P₂c₃₁m |
|            | 162.7.1309 | P₂c₃₁m' | P₂c₃₁c |

**158.1.1289** P₃c₁  
| 163.1.1310 | P₃₁c |

| 158.2.1290 | P₃c₁₁' | 163.2.1311 | P₃₁c₁' |
| 158.3.1291 | P₃c'₁ | 163.3.1312 | P₃'₁c |

**159.1.1292** P₃₁c  
| 163.4.1313 | P₃'₁c' |

TABLE 1.4 - 3D - 31
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**HEXAGONAL SYSTEM**

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**TABLE 1.4 - 3D - 32**
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TABLE 1.4 - 3D - 34
| 186.5.1438 | P\textsubscript{6}\textsubscript{3} m'c' | 190.2.1459 | P6\textsubscript{2}c1' |
| 187.1.1439 | P6m2 | 190.3.1460 | P6'2'c |
| 187.2.1440 | P6m21' | 190.4.1461 | P6'2c' |
| 187.3.1441 | P\bar{6}m'2 | 190.5.1462 | P6'2'c' |
| 187.4.1442 | P6'm2' | 191.1.1463 | P6/mmm |
| 187.5.1443 | P6m'2' | 191.2.1464 | P6/mmm1' |
| 187.6.1444 | P\textsubscript{2}c \bar{6}m2 | P\textsubscript{c} \bar{6}m2 | 191.3.1465 | P6/m'mm |
| 187.7.1445 | P\textsubscript{2}c \bar{6}'m'2 | P\textsubscript{c} \bar{6}c2 | 191.4.1466 | P6'/mm'm |
| 188.1.1446 | P6c2 | 191.5.1467 | P6'/mmm' |
| 188.2.1447 | P\bar{6}c21' | 191.6.1468 | P6'/m'm'm |
| 188.3.1448 | P\textsubscript{6}c'2 | 191.7.1469 | P6'/m'm'm' |
| 188.4.1449 | P\textsubscript{6}'c2' | 191.8.1470 | P6/mm'm' |
| 188.5.1450 | P\textsubscript{6}c'2' | 191.9.1471 | P6/m'm'm' |
| 189.1.1451 | P62m | 191.10.1472 | P\textsubscript{2}c 6/mmm | P\textsubscript{c} 6/mmm |
| 189.2.1452 | P\bar{6}2m1' | 191.11.1473 | P\textsubscript{2}c 6'/mm'm | P\textsubscript{c} 6\textsubscript{3} /mcm |
| 189.3.1453 | P6'2'm | 191.12.1474 | P\textsubscript{2}c 6'/mmm' | P\textsubscript{c} 6\textsubscript{3} /mmc |
| 189.4.1454 | P6'2'm' | 191.13.1475 | P\textsubscript{2}c 6/m'm'm' | P\textsubscript{c} 6/mcc |
| 189.5.1455 | P\bar{6}2'm' | 192.1.1476 | P6/mcc |
| 189.6.1456 | P\textsubscript{2}c \bar{6}2m | P\textsubscript{c} \bar{6}2m | 192.2.1477 | P6/mcc1' |
| 189.7.1457 | P\textsubscript{2}c \bar{6}'2m' | P\textsubscript{c} \bar{6}2c | 192.3.1478 | P6/m'cc |
| 190.1.1458 | P6\textsubscript{2}c | 192.4.1479 | P6'/mc'c |

**TABLE 1.4 - 3D - 35**
| 192.5.1480 | P6'/mcc' | 194.9.1502 | P6₃/m'm'c' |
| 192.6.1481 | P6'/m'c'c | | |
| 192.7.1482 | P6'/m'cc' | | |
| 192.8.1483 | P6/mc'c' | **CUBIC SYSTEM** | |
| 192.9.1484 | P6/m'c'c' | | |
| **193.1.1485** | **P6₃/mcm** | | |
| 193.2.1486 | P6₃/mcm1' | **196.1.1506** | F23 |
| 193.3.1487 | P6₃/m'cm | | |
| 193.4.1488 | P6₃/mc'm | | |
| 193.5.1489 | P6₃/mcm' | **197.1.1508** | I23 |
| 193.6.1490 | P6₃/m'c'm | | |
| 193.7.1491 | P6₃/m'cm' | | |
| 193.8.1492 | P6₃/mc'm' | **198.1.1511** | P2,3 |
| 193.9.1493 | P6₃/m'c'm' | | |
| **194.1.1494** | **P6₃/mmc** | | |
| 194.2.1495 | P6₃/mmc1' | **199.1.1513** | I2,3 |
| 194.3.1496 | P6₃/m'mc | | |
| 194.4.1497 | P6₃/m'mc' | | |
| 194.5.1498 | P6₃/mm'm'c | **200.1.1516** | Pm̅3 |
| 194.6.1499 | P6₃/m'm'm'c | | |
| 194.7.1500 | P6₃/m'm'mc' | | |
| 194.8.1501 | P6₃/mm'm'c' | **200.4.1519** | P F m̅3 |
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**TABLE 1.4 - 3D - 36**
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<td>P$<em>{4</em>{2}}$ 321'</td>
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TABLE 1.4 - 3D - 37
TABLE 1. 4 - 3D - 38

211.5.1560  \( I_p, 4'32' \)  \( P_1 4_2 32 \)  \( 217.1.1580  \( I\bar{4}3m \)

212.1.1561  \( P_{43} 32 \)  \( 217.2.1581  I\bar{4}3m1' \)

212.2.1562  \( P_{43} 321' \)  \( 217.3.1582  I4'3m' \)

212.3.1563  \( P_{43} 32' \)  \( 217.4.1583  I_p \bar{4}3m \)  \( P_4 43m \)

213.1.1564  \( P_{43} 32 \)  \( 218.1.1585  P_{43n} \)

213.2.1565  \( P_{43} 321' \)  \( 218.2.1586  P_{43} 3n1' \)

213.3.1566  \( P_{43} 32' \)  \( 218.3.1587  P_{43} 3n' \)

214.1.1567  \( I4, 32 \)  \( 219.1.1588  F_{43c} \)

214.2.1568  \( I4, 321' \)  \( 219.2.1589  F_{43c1'} \)

214.3.1569  \( I4, 32' \)  \( 219.3.1590  F4'3c' \)

214.4.1570  \( I_p 4, 32 \)  \( P_1 4_3 32 \)  \( 219.4.1583  I43d \)

214.5.1571  \( I_p 4_1, 32' \)  \( P_1 4_1 32 \)  \( 220.1.1591  I43d \)

215.1.1572  \( P_{43m} \)  \( 220.2.1592  I\bar{4}3d1' \)

215.2.1573  \( P_{43m1'} \)  \( 220.3.1593  I4'3d' \)

215.3.1574  \( P_{43m'} \)  \( 221.1.1594  P_{m\bar{3}m} \)

215.4.1575  \( P_{r43m} \)  \( F_s 43m \)  \( 221.2.1595  P_{m\bar{3}m1'} \)

215.5.1576  \( P_{r43m'} \)  \( F_s 43c \)  \( 221.3.1596  P_{m\bar{3}m'} \)

216.1.1577  \( F_{43m} \)  \( 221.4.1597  P_{m\bar{3}m} \)

216.2.1578  \( F_{43m1'} \)  \( 221.5.1598  P_{m\bar{3}m} \)

216.3.1579  \( F_{43m'} \)  \( 221.6.1599  P_{F} m3m \)  \( F_s m3m \)

217.1.1580  \( I\bar{4}3m \)

217.2.1581  \( I\bar{4}3m1' \)

217.3.1582  \( I4'3m' \)

217.4.1583  \( I_p \bar{4}3m \)  \( P_4 43m \)

217.5.1584  \( I_p 4'3m' \)  \( P_4 43n \)

218.1.1585  \( P_{43n} \)

218.2.1586  \( P_{43} 3n1' \)

218.3.1587  \( P_{43} 3n' \)

219.1.1588  \( F_{43c} \)

219.2.1589  \( F_{43c1'} \)

219.3.1590  \( F4'3c' \)

219.4.1583  \( I43d \)

220.1.1591  \( I43d \)

220.2.1592  \( I\bar{4}3d1' \)

220.3.1593  \( I4'3d' \)

221.1.1594  \( P_{m\bar{3}m} \)

221.2.1595  \( P_{m\bar{3}m1'} \)

221.3.1596  \( P_{m\bar{3}m'} \)

221.4.1597  \( P_{m\bar{3}m} \)

221.5.1598  \( P_{m\bar{3}m} \)

221.6.1599  \( P_{F} m3m \)  \( F_s m3m \)

221.7.1600  \( P_{F} m3m' \)  \( F_s m3c \)
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<th>Description</th>
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<tr>
<td>222.2.1602</td>
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<td>222.3.1603</td>
<td>Pn'3'n</td>
<td>226.2.1624</td>
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<td>222.4.1604</td>
<td>Pn3n'</td>
<td>226.3.1625</td>
<td>Fm3'3'c</td>
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<td>Pn'3'n'</td>
<td>226.4.1626</td>
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<td>223.1.1606</td>
<td>Pm3n</td>
<td>226.5.1627</td>
<td>Fm3'3'c'</td>
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<tr>
<td>223.2.1607</td>
<td>Pm3n1'</td>
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<td>223.3.1608</td>
<td>Pm'3'n</td>
<td>227.2.1629</td>
<td>Fd3m1'</td>
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<td>223.4.1609</td>
<td>Pm3n'</td>
<td>227.3.1630</td>
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<td>227.4.1631</td>
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<td>224.1.1611</td>
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<td>227.5.1632</td>
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<td>224.2.1612</td>
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<td>224.3.1613</td>
<td>Pn'3'm</td>
<td>228.2.1634</td>
<td>Fd3c1'</td>
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<td>224.4.1614</td>
<td>Pn3m'</td>
<td>228.3.1635</td>
<td>Fd'3'c</td>
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<tr>
<td>224.5.1615</td>
<td>Pn'3'm'</td>
<td>228.4.1636</td>
<td>Fd3c'</td>
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<td>224.6.1616</td>
<td>P_f n3m</td>
<td>228.5.1637</td>
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<td>224.7.1617</td>
<td>P_f n3m'</td>
<td>F_s d3m</td>
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<td>225.2.1619</td>
<td>Fm3m1'</td>
<td>229.2.1639</td>
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<td>225.3.1620</td>
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TABLE 1.4 - 3D - 39
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<td>Pₚm₃m</td>
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<td>Pₚn₃m</td>
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<td>229.8.1645</td>
<td>Iₚm₃m'</td>
<td>Pₚm₃n</td>
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<td>229.9.1646</td>
<td>Iₚm'₃'m'</td>
<td>Pₚn₃n</td>
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<td>230.3.1649</td>
<td>Iₚ'₃'d</td>
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<td>Iₚ₃d'</td>
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TABLE 1.4 - 3D - 40
### Table 1.4 - 2D

**Table 1.4 - 2D**

**Two-dimensional**: Magnetic space group symbols of Table 1.1-2D compared with the one-dimensional black and white symbols given by Belov and Tarkhova (BT) (1956).

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<tr>
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<td>p11'</td>
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<td>p2'm'g'</td>
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<tr>
<td>1.3.3 p2a1</td>
<td>p'1</td>
<td>7.5.35</td>
<td>p2'mg'</td>
</tr>
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<td></td>
<td>7.6.36</td>
<td>p2a2m'g'</td>
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<td>p2</td>
<td>7.7.37</td>
<td>p2b2mg</td>
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<td>2.3.6 p2'11</td>
<td>p2'</td>
<td>8.1.38</td>
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<td>pmm21'</td>
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<td>pm'm'</td>
<td>11.7.59</td>
<td>p_p4m'</td>
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**TABLE 1.4 - 2D - 1**
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**Table 1.4 - 1D**

**One-Dimensional:** Magnetic space group symbols of Table 1.1-1D compared with the one-dimensional black and white symbols given by Niggli (1964).

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### Table 2.2.3-3D Graphical Symbols

#### Three-Dimensional Magnetic Space Groups

**2.2.3.1 Symmetry axes parallel to the plane of projection**

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<th>Graphical symbol</th>
<th>Screw vector of a right-handed screw rotation in units of the shortest non-primed translation vector parallel to the axis</th>
<th>Printed symbol</th>
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<td>Twofold unprimed rotation axis,</td>
<td><img src="image" alt="twofold symbol" /></td>
<td>None</td>
<td>2</td>
</tr>
<tr>
<td>Twofold primed rotation axis</td>
<td><img src="image" alt="twofold symbol" /></td>
<td>None</td>
<td>2'</td>
</tr>
<tr>
<td>Twofold unprimed screw axis, 2 sub 1</td>
<td><img src="image" alt="twofold symbol" /></td>
<td>1/2</td>
<td>2,</td>
</tr>
<tr>
<td>Twofold primed screw axis, 2 sub 1 primed</td>
<td><img src="image" alt="twofold symbol" /></td>
<td>1/2</td>
<td>2, primed</td>
</tr>
<tr>
<td>Fourfold unprimed rotation axis</td>
<td><img src="image" alt="fourfold symbol" /></td>
<td>None</td>
<td>4</td>
</tr>
<tr>
<td>Fourfold primed rotation axis</td>
<td><img src="image" alt="fourfold symbol" /></td>
<td>None</td>
<td>4'</td>
</tr>
<tr>
<td>Fourfold unprimed screw axis, 4 sub 1</td>
<td><img src="image" alt="fourfold symbol" /></td>
<td>1/4</td>
<td>4,</td>
</tr>
<tr>
<td>Fourfold primed screw axis, 4 sub 1 primed</td>
<td><img src="image" alt="fourfold symbol" /></td>
<td>1/4</td>
<td>4, primed</td>
</tr>
<tr>
<td>Fourfold unprimed screw axis, 4 sub 2</td>
<td><img src="image" alt="fourfold symbol" /></td>
<td>1/2</td>
<td>4,</td>
</tr>
<tr>
<td>Fourfold primed screw axis, 4 sub 2 primed</td>
<td><img src="image" alt="fourfold symbol" /></td>
<td>1/2</td>
<td>4, primed</td>
</tr>
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### 2.2.3.2 Symmetry axes normal to the plane of projection

<table>
<thead>
<tr>
<th>Symmetry Axis or symmetry point</th>
<th>Graphical symbol</th>
<th>Screw vector of a right-handed screw rotation in units of the shortest non-primed translation vector parallel to the axis.</th>
<th>Printed symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Identity</td>
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<td>None</td>
<td>1</td>
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<tr>
<td>Twofold unprimed rotation axis, 2</td>
<td></td>
<td>None</td>
<td>2</td>
</tr>
<tr>
<td>Twofold primed rotation axis, 2 primed</td>
<td></td>
<td>None</td>
<td>2'</td>
</tr>
<tr>
<td>Twofold unprimed screw axis, 2 sub 1</td>
<td></td>
<td>1/2</td>
<td>2_1</td>
</tr>
<tr>
<td>Twofold primed screw axis, 2 sub 1 primed</td>
<td></td>
<td>1/2</td>
<td>2'_1</td>
</tr>
<tr>
<td>Axis Type</td>
<td>Symbol</td>
<td>Prime</td>
<td>Factor</td>
</tr>
<tr>
<td>-------------------</td>
<td>-----------------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>Threefold unprimed</td>
<td><img src="image" alt="Triangle" /></td>
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<td>1/3</td>
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<tr>
<td>Threefold primed</td>
<td><img src="image" alt="Triangle" /></td>
<td>None</td>
<td>1/3</td>
</tr>
<tr>
<td>Threefold unprimed</td>
<td><img src="image" alt="Triangle" /></td>
<td>2/3</td>
<td>2/3</td>
</tr>
<tr>
<td>Threefold primed</td>
<td><img src="image" alt="Triangle" /></td>
<td>2/3</td>
<td>2/3</td>
</tr>
<tr>
<td>Fourfold unprimed</td>
<td><img src="image" alt="Square" /></td>
<td>None</td>
<td>1/4</td>
</tr>
<tr>
<td>Fourfold primed</td>
<td><img src="image" alt="Square" /></td>
<td>None</td>
<td>1/4</td>
</tr>
<tr>
<td>Fourfold unprimed</td>
<td><img src="image" alt="Square" /></td>
<td>1/4</td>
<td>1/4</td>
</tr>
<tr>
<td>Fourfold primed</td>
<td><img src="image" alt="Square" /></td>
<td>1/4</td>
<td>1/4</td>
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Table 2.2.3 - 3
<table>
<thead>
<tr>
<th>Axis Type</th>
<th>Description</th>
<th>Axis Order</th>
<th>Subscript</th>
<th>Prime</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fourfold unprimed</td>
<td>Screw axis, 4 sub 2</td>
<td>1/2</td>
<td>4</td>
<td>$4_2$</td>
</tr>
<tr>
<td>Fourfold primed</td>
<td>Screw axis, 4 sub 2 primed</td>
<td>1/2</td>
<td>4</td>
<td>$4_2'$</td>
</tr>
<tr>
<td>Fourfold unprimed</td>
<td>Screw axis, 4 sub 3</td>
<td>3/4</td>
<td>4</td>
<td>$4_3$</td>
</tr>
<tr>
<td>Fourfold primed</td>
<td>Screw axis, 4 sub 3 primed</td>
<td>3/4</td>
<td>4</td>
<td>$4_3'$</td>
</tr>
<tr>
<td>Sixfold unprimed</td>
<td>Rotation axis, 6</td>
<td>None</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>Sixfold primed</td>
<td>Rotation axis, 6 primed</td>
<td>None</td>
<td>6</td>
<td>$6'$</td>
</tr>
<tr>
<td>Sixfold unprimed</td>
<td>Screw axis, 6 sub 1</td>
<td>1/6</td>
<td>6</td>
<td>$6_1$</td>
</tr>
<tr>
<td>Sixfold primed</td>
<td>Screw axis, 6 sub 1 primed</td>
<td>1/6</td>
<td>6</td>
<td>$6_1'$</td>
</tr>
<tr>
<td>Sixfold unprimed</td>
<td>Screw axis, 6 sub 2</td>
<td>1/3</td>
<td>6</td>
<td>$6_2$</td>
</tr>
<tr>
<td>Sixfold primed</td>
<td>Screw axis, 6 sub 2 primed</td>
<td>1/3</td>
<td>6</td>
<td>$6_2'$</td>
</tr>
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Table 2.2.3 - 4
<table>
<thead>
<tr>
<th>Symmetry Type</th>
<th>Axis Type</th>
<th>Factor</th>
<th>Letter</th>
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<tbody>
<tr>
<td>Sixfold unprimed</td>
<td>screw axis</td>
<td>1/2</td>
<td>$6_3$</td>
</tr>
<tr>
<td>Sixfold primed</td>
<td>screw axis</td>
<td>1/2</td>
<td>$6_3'$</td>
</tr>
<tr>
<td>Sixfold unprimed</td>
<td>screw axis</td>
<td>2/3</td>
<td>$6_4$</td>
</tr>
<tr>
<td>Sixfold primed</td>
<td>screw axis</td>
<td>2/3</td>
<td>$6_4'$</td>
</tr>
<tr>
<td>Sixfold unprimed</td>
<td>screw axis</td>
<td>5/6</td>
<td>$6_5$</td>
</tr>
<tr>
<td>Sixfold primed</td>
<td>screw axis</td>
<td>5/6</td>
<td>$6_5'$</td>
</tr>
<tr>
<td>Unprimed center of symmetry,</td>
<td>None</td>
<td></td>
<td>$\bar{1}$</td>
</tr>
<tr>
<td>unprimed inversion center,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 bar</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primed center of symmetry,</td>
<td>None</td>
<td></td>
<td>$\bar{1}'$</td>
</tr>
<tr>
<td>primed inversion center,</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 bar primed</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Twofold unprimed rotation</td>
<td>None</td>
<td></td>
<td>$2, \bar{1} = 2/m$</td>
</tr>
<tr>
<td>axis with unprimed center of</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>symmetry</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Twofold primed rotation axis</td>
<td>None</td>
<td></td>
<td>$2', \bar{1}' = 2'/m'$</td>
</tr>
<tr>
<td>axis with unprimed center of</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>symmetry</td>
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Table 2.2.3 - 5
<table>
<thead>
<tr>
<th>Description</th>
<th>Symbol</th>
<th>Image</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Twofold unprimed rotation axis with primed center of symmetry</td>
<td>2, ( \overline{1}' = \frac{2}{m'} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Twofold primed rotation axis with primed center of symmetry</td>
<td>2', ( \overline{1}' = \frac{2'}{m} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Twofold unprimed screw axis with unprimed center of symmetry</td>
<td>( \frac{1}{2} )</td>
<td>2₁, ( \overline{\tau} )</td>
<td></td>
</tr>
<tr>
<td>Twofold primed screw axis with unprimed center of symmetry</td>
<td>( \frac{1}{2} )</td>
<td>2₁', ( \overline{\tau} )</td>
<td></td>
</tr>
<tr>
<td>Twofold unprimed screw axis with primed center of symmetry</td>
<td>( \frac{1}{2} )</td>
<td>2₁, ( \overline{1}' )</td>
<td></td>
</tr>
<tr>
<td>Twofold primed screw axis with primed center of symmetry</td>
<td>( \frac{1}{2} )</td>
<td>2₁', ( \overline{1}' )</td>
<td></td>
</tr>
<tr>
<td>Twofold unprimed screw axis, twofold unprimed rotation axis,</td>
<td>( \frac{1}{2} )</td>
<td>2₁,2'</td>
<td></td>
</tr>
<tr>
<td>and primed and unprimed centers of symmetry</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Twofold unprimed screw axis, twofold primed rotation axis, and</td>
<td>( \frac{1}{2} )</td>
<td>2₁,2',1,( \overline{1}' )</td>
<td></td>
</tr>
<tr>
<td>primed and unprimed centers of symmetry</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Twofold unprimed screw axis, twofold primed rotation axis, and</td>
<td>( \frac{1}{2} )</td>
<td>2₁,2',( \overline{1}',\overline{\tau} )</td>
<td></td>
</tr>
<tr>
<td>primed and unprimed centers of symmetry</td>
<td></td>
<td></td>
<td></td>
</tr>
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</table>

Table 2.2.3 - 6
<table>
<thead>
<tr>
<th>Symmetry Operation</th>
<th>Description</th>
<th>Image</th>
<th>Center of Symmetry</th>
<th>Symmetry Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Threefold unprimed</td>
<td>Rotation axis with unprimed</td>
<td><img src="triangle.png" alt="Triangle" /></td>
<td>None</td>
<td>$3, \bar{1} = \bar{3}$</td>
</tr>
<tr>
<td>Threefold unprimed</td>
<td>Rotation axis with primed</td>
<td><img src="triangle.png" alt="Triangle" /></td>
<td>None</td>
<td>$3, \bar{1}' = \bar{3}'$</td>
</tr>
<tr>
<td>Threefold unprimed</td>
<td>Rotation axis with primed and</td>
<td><img src="triangle.png" alt="Triangle" /></td>
<td>None</td>
<td>$3, \bar{1}', \bar{1}$</td>
</tr>
<tr>
<td>Fourfold unprimed</td>
<td>Rotation axis with unprimed</td>
<td><img src="square.png" alt="Square" /></td>
<td>None</td>
<td>$4, \bar{1} = 4/m$</td>
</tr>
<tr>
<td>Fourfold primed</td>
<td>Rotation axis with unprimed</td>
<td><img src="square.png" alt="Square" /></td>
<td>None</td>
<td>$4', \bar{1} = 4'/m$</td>
</tr>
<tr>
<td>Fourfold unprimed</td>
<td>Rotation axis with primed</td>
<td><img src="square.png" alt="Square" /></td>
<td>None</td>
<td>$4, \bar{1}' = 4/m'$</td>
</tr>
<tr>
<td>Fourfold primed</td>
<td>Rotation axis with primed</td>
<td><img src="square.png" alt="Square" /></td>
<td>None</td>
<td>$4, \bar{1}' = 4/m'$</td>
</tr>
<tr>
<td>Fourfold unprimed</td>
<td>Screw axis with unprimed</td>
<td><img src="square.png" alt="Square" /></td>
<td>1/2</td>
<td>$4_2, \bar{1}$</td>
</tr>
<tr>
<td>Fourfold primed</td>
<td>Screw axis with unprimed</td>
<td><img src="square.png" alt="Square" /></td>
<td>1/2</td>
<td>$4_{2}', \bar{1}$</td>
</tr>
<tr>
<td>Fourfold unprimed</td>
<td>Screw axis with primed</td>
<td><img src="square.png" alt="Square" /></td>
<td>1/2</td>
<td>$4_{2}, \bar{1}'$</td>
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Table 2.2.3 - 7
<table>
<thead>
<tr>
<th>Description</th>
<th>Diagram</th>
<th>Value</th>
<th>Notation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fourfold primed screw axis with primed center of symmetry</td>
<td><img src="image1" alt="Diagram" /></td>
<td>1/2</td>
<td>$4_2', \overline{1}'$</td>
</tr>
<tr>
<td>Fourfold primed screw axis with fourfold unprimed rotation axis</td>
<td><img src="image2" alt="Diagram" /></td>
<td>1/2</td>
<td>$4_2', 4$</td>
</tr>
<tr>
<td>Fourfold unprimed screw axis with fourfold primed rotation axis</td>
<td><img src="image3" alt="Diagram" /></td>
<td>1/2</td>
<td>$4_2, 4'$</td>
</tr>
<tr>
<td>Fourfold primed screw axis, fourfold unprimed rotation axis and primed and unprimed and center of symmetry</td>
<td><img src="image4" alt="Diagram" /></td>
<td>1/2</td>
<td>$4_2', 4, \overline{1}', \overline{1}$</td>
</tr>
<tr>
<td>Fourfold unprimed screw axis, fourfold primed rotation axis, and primed and unprimed and center of symmetry</td>
<td><img src="image5" alt="Diagram" /></td>
<td>1/2</td>
<td>$4_2, 4', \overline{1}', \overline{1}$</td>
</tr>
<tr>
<td>Fourfold unprimed screw axis 4 sub 1 and fourfold primed screw axis 4 sub 3 prime</td>
<td><img src="image6" alt="Diagram" /></td>
<td>1/4, 3/4</td>
<td>$4_1, 4_3'$</td>
</tr>
<tr>
<td>Fourfold primed screw axis 4 sub 1 prime and fourfold unprimed screw axis 4 sub 3</td>
<td><img src="image7" alt="Diagram" /></td>
<td>1/4, 3/4</td>
<td>$4_1', 4_3$</td>
</tr>
<tr>
<td>Unprimed inversion axis 4 bar</td>
<td><img src="image8" alt="Diagram" /></td>
<td>None</td>
<td>$\overline{4}, 2 = \overline{4}$</td>
</tr>
<tr>
<td>Primed inversion axis 4 bar prime</td>
<td><img src="image9" alt="Diagram" /></td>
<td>None</td>
<td>$\overline{4}', 2 = \overline{4}'$</td>
</tr>
</tbody>
</table>
| Primed and unprimed inversion axes 4 bar and 4 bar prime, and primed twofold screw axis | ![Diagram](image10)      | 1/2      | $\overline{4}, 2 = \overline{4}$  
|                                                                              |                          |          | $\overline{4}', 2 = \overline{4}'$  
|                                                                              |                          |          | $2_1'$        |

Table 2.2.3 - 8
<table>
<thead>
<tr>
<th>Symmetry Operation</th>
<th>Center of Symmetry</th>
<th>6, $\overline{1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sixfold unprimed rotation axis with unprimed center</td>
<td>None</td>
<td>$6, \overline{1} = 6/m$</td>
</tr>
<tr>
<td>of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold primed rotation axis with unprimed center</td>
<td>None</td>
<td>$6', \overline{1} = 6'/m$</td>
</tr>
<tr>
<td>of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold unprimed rotation axis with primed center</td>
<td>None</td>
<td>$6, \overline{1}' = 6/m'$</td>
</tr>
<tr>
<td>of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold primed rotation axis with primed center</td>
<td>None</td>
<td>$6', \overline{1}' = 6'/m'$</td>
</tr>
<tr>
<td>of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold unprimed screw axis 6 sub 3 with unprimed</td>
<td>1/2</td>
<td>$6_3, \overline{1}$</td>
</tr>
<tr>
<td>center of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold primed screw axis 6 sub 3 prime with</td>
<td>1/2</td>
<td>$6_3', \overline{1}$</td>
</tr>
<tr>
<td>unprimed center of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold unprimed screw axis 6 sub 3 with primed</td>
<td>1/2</td>
<td>$6_3, \overline{1}'$</td>
</tr>
<tr>
<td>center of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold primed screw axis 6 sub 3 prime with</td>
<td>1/2</td>
<td>$6_3', \overline{1}'$</td>
</tr>
<tr>
<td>primed center of symmetry</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold unprimed rotation axis, sixfold primed screw</td>
<td>1/2</td>
<td>$6_3', 6$</td>
</tr>
<tr>
<td>axis 6 sub 3 prime</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sixfold primed rotation axis, sixfold unprimed screw</td>
<td>1/2</td>
<td>$6_3, 6'$</td>
</tr>
<tr>
<td>axis 6 sub 3</td>
<td></td>
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</tr>
</tbody>
</table>

Table 2.2.3 - 9
Table 2.2.3 - 10

Sixfold unprimed rotation axis, sixfold primed screw axis 6 sub 3 prime, with primed and unprimed centers of symmetry

Sixfold primed rotation axis, sixfold unprimed screw axis 6 sub 3, with primed and unprimed centers of symmetry

Unprimed inversion axis
6 bar

Primed inversion axis
6 bar prime

Primed and unprimed inversion axes, 6 bar prime and 6 bar

Primed and unprimed centers of symmetry

2.2.3.3 Symmetry planes normal to the plane of projection

<table>
<thead>
<tr>
<th>Symmetry plane</th>
<th>Graphical symbol</th>
<th>Glide vector in units of unprimed lattice translation parallel and normal to the projection plane</th>
<th>Printed symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unprimed reflection plane</td>
<td>![Graphic]</td>
<td>None</td>
<td>m</td>
</tr>
<tr>
<td>Primed reflection plane</td>
<td>![Graphic]</td>
<td>None</td>
<td>m'</td>
</tr>
<tr>
<td>Unprimed axial glide plane</td>
<td>![Graphic]</td>
<td>1/2 along line parallel to projection plane</td>
<td>a,b</td>
</tr>
<tr>
<td>Glide Plane Type</td>
<td>Glide Component Details</td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------------------</td>
<td>----------------------------------------------------------------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primed Axial Glide Plane</td>
<td>1/2 along line parallel to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unprimed Axial Glide Plane</td>
<td>1/2 along line normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primed Axial Glide Plane</td>
<td>1/2 along line normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unprimed Diagonal Glide Plane</td>
<td>One glide plane with two components: 1/2 along line parallel to projection plane and 1/2 normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primed Diagonal Glide Plane</td>
<td>One glide plane with two components: 1/2 along line parallel to projection plane and 1/2 normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unprimed Diamond Glide Plane</td>
<td>One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow and 1/4 up normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primed Diamond Glide Plane</td>
<td>One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow and 3/4 up normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unprimed Diamond Glide Plane</td>
<td>One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow and 3/4 up normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primed Diamond Glide Plane</td>
<td>One glide plane with two components: 1/4 along line parallel to projection plane in direction of arrow and 3/4 up normal to projection plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unprimed Axial Glide Planes</td>
<td>Two glide planes each with one component: 1/2 along line parallel to projection plane; 1/2 normal to projection plane</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### 2.2.3.4 Symmetry planes parallel to the plane of projection

<table>
<thead>
<tr>
<th>Symmetry plane</th>
<th>Graphical symbol</th>
<th>Glide vector in units of unprimed lattice translation parallel to the projection plane</th>
<th>Printed symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unprimed reflection plane</td>
<td><img src="image" alt="Graphical Symbol" /></td>
<td>None 1/2 along direction parallel to arrow</td>
<td>m</td>
</tr>
<tr>
<td>Primed reflection plane</td>
<td><img src="image" alt="Graphical Symbol" /></td>
<td>None 1/2 along direction parallel to arrow</td>
<td>m'</td>
</tr>
<tr>
<td>Unprimed axial glide plane</td>
<td><img src="image" alt="Graphical Symbol" /></td>
<td>1/2 along direction parallel to arrow</td>
<td>a,b</td>
</tr>
<tr>
<td>Primed axial glide plane</td>
<td><img src="image" alt="Graphical Symbol" /></td>
<td>1/2 along direction parallel to arrow</td>
<td>a',b'</td>
</tr>
<tr>
<td>Unprimed double glide plane</td>
<td><img src="image" alt="Graphical Symbol" /></td>
<td>Two glide planes each with one component 1/2 along directions parallel to the two arrows</td>
<td></td>
</tr>
</tbody>
</table>
### Table 2.2.3 - 13

<table>
<thead>
<tr>
<th>Symmetry plane</th>
<th>Graphical symbol</th>
<th>Screw vector of a right-handed screw rotation in units of the shortest unprimed lattice translation parallel to the axis</th>
<th>Printed symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unprimed twofold rotation axis parallel to a face diagonal of the cube</td>
<td><img src="image" alt="Diagram" /></td>
<td>None</td>
<td>2</td>
</tr>
</tbody>
</table>

#### 2.2.3.5 Symmetry axes inclined to the plane of projection (in cubic magnetic space groups only)

- **Primed double glide plane**: Two glide planes each with one component 1/2 along directions parallel to the two arrows.
- **Unprimed diagonal glide plane**: 1/2 along direction parallel to arrow.
- **Primed diagonal glide plane**: 1/2 along direction parallel to arrow.
- **Unprimed double glide plane and unprimed diagonal glide plane**: Three glide planes each with one component 1/2 along directions parallel to the three arrows.
- **Primed double glide plane and primed diagonal glide plane**: Three glide planes each with one component 1/2 along directions parallel to the three arrows.
- **Unprimed double diagonal glide planes**: Two glide planes each with one component 1/2 along directions parallel to the two arrows.
- **Primed double diagonal glide planes**: Two glide planes each with one component 1/2 along directions parallel to the two arrows.
<table>
<thead>
<tr>
<th>Description</th>
<th>Symbol 1</th>
<th>Symbol 2</th>
<th>Prime</th>
<th>Rotation Axis</th>
<th>Other Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primed twofold rotation axis parallel to a face diagonal of the cube</td>
<td></td>
<td></td>
<td>None</td>
<td>2'</td>
<td></td>
</tr>
<tr>
<td>Unprimed twofold screw axis 2 sub 1 parallel to a face diagonal of the cube</td>
<td></td>
<td></td>
<td>1/2</td>
<td>2&lt;sub&gt;1&lt;/sub&gt;</td>
<td></td>
</tr>
<tr>
<td>Primed twofold screw axis 2 sub 1 prime parallel to a face diagonal of the cube</td>
<td></td>
<td></td>
<td>1/2</td>
<td>2&lt;sub&gt;1'&lt;/sub&gt;</td>
<td></td>
</tr>
<tr>
<td>Unprimed threefold rotation axis parallel to a body diagonal of the cube</td>
<td></td>
<td></td>
<td>None</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Unprimed threefold screw axis 3 sub 1 parallel to a body diagonal of the cube</td>
<td></td>
<td></td>
<td>1/3</td>
<td>3&lt;sub&gt;1&lt;/sub&gt;</td>
<td></td>
</tr>
<tr>
<td>Primed threefold screw axis 3 sub 1 prime parallel to a body diagonal of the cube</td>
<td></td>
<td></td>
<td>1/3</td>
<td>3&lt;sub&gt;1'&lt;/sub&gt;</td>
<td></td>
</tr>
<tr>
<td>Unprimed threefold screw axis 3 sub 2 parallel to a body diagonal of the cube</td>
<td></td>
<td></td>
<td>2/3</td>
<td>3&lt;sub&gt;2&lt;/sub&gt;</td>
<td></td>
</tr>
<tr>
<td>Primed threefold screw axis 3 sub 2 prime parallel to a body diagonal of the cube</td>
<td></td>
<td></td>
<td>2/3</td>
<td>3&lt;sub&gt;2'&lt;/sub&gt;</td>
<td></td>
</tr>
<tr>
<td>Unprimed inversion axis 3 bar parallel to a body diagonal of the cube</td>
<td></td>
<td></td>
<td>None</td>
<td>3,1 = 3</td>
<td></td>
</tr>
</tbody>
</table>
### 2.2.3.6 Symmetry planes inclined to the plane of projection (in cubic magnetic space groups only)

<table>
<thead>
<tr>
<th>Symmetry Plane Symbol</th>
<th>Graphical symbol for planes normal to [011] and [01(\overline{1})]; [101] and [10(\overline{1})]</th>
<th>Glide vectors in units of unprimed lattice translation for planes normal to [011] and [01(\overline{1})]; [101] and [10(\overline{1})]</th>
<th>Printed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unprimed Reflection plane</td>
<td><img src="image1" alt="Diagram" /></td>
<td>None</td>
<td>m</td>
</tr>
<tr>
<td>Primed Reflection plane</td>
<td><img src="image2" alt="Diagram" /></td>
<td>None</td>
<td>m'</td>
</tr>
<tr>
<td>Unprimed axial glide plane</td>
<td><img src="image3" alt="Diagram" /></td>
<td>1/2 along [100]</td>
<td>a,b</td>
</tr>
<tr>
<td>Primed axial glide plane</td>
<td><img src="image4" alt="Diagram" /></td>
<td>1/2 along [100]</td>
<td>a',b'</td>
</tr>
<tr>
<td>Unprimed axial glide plane</td>
<td><img src="image5" alt="Diagram" /></td>
<td>1/2 along [01(\overline{1})] or [101]</td>
<td></td>
</tr>
<tr>
<td>Unprimed axial glide plane</td>
<td><img src="image6" alt="Diagram" /></td>
<td>1/2 along [01(\overline{1})] or [101]</td>
<td></td>
</tr>
</tbody>
</table>
Table 2.2.3 - 16

<table>
<thead>
<tr>
<th>Unprimed double glide plane</th>
<th>Two glide vectors: 1/2 along [100] and 1/2 along [011] or [011]</th>
<th>Two glide vectors: 1/2 along [010] and 1/2 along [101] or [101]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primed double glide plane</td>
<td>Two glide vectors: 1/2 along [100] and 1/2 along [011] or [011]</td>
<td>Two glide vectors: 1/2 along [010] and 1/2 along [101] or [101]</td>
</tr>
<tr>
<td>Unprimed diagonal glide plane</td>
<td>1/2 along [111] or [111]</td>
<td>1/2 along [111] or [111]</td>
</tr>
<tr>
<td>Primed diagonal glide plane</td>
<td>1/2 along [111] or [111]</td>
<td>1/2 along [111] or [111]</td>
</tr>
<tr>
<td>Unprimed diamond glide plane</td>
<td>1/2 along [111] or [111]</td>
<td>1/2 along [111] or [111]</td>
</tr>
<tr>
<td></td>
<td>1/2 along [111] or [111]</td>
<td>1/2 along [111] or [111]</td>
</tr>
</tbody>
</table>
Table 2.2.3 - 17

<table>
<thead>
<tr>
<th>Primed diamond glide plane</th>
<th>1/2 along [111] or [111]</th>
<th>1/2 along [111] or [111]</th>
<th>d'</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Unprimed axial glide planes</th>
<th>Two glide vectors: 1/2 along [100] and 1/2 along [011]</th>
<th>Two glide vectors: 1/2 along [010] and 1/2 along [101]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Unprimed axial glide planes</th>
<th>Two glide vectors: 1/2 along [100] and 1/2 along [011]</th>
<th>Two glide vectors: 1/2 along [010] and 1/2 along [101]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Primed axial glide planes</th>
<th>Two glide vectors: 1/2 along [100] and 1/2 along [011]</th>
<th>Two glide vectors: 1/2 along [010] and 1/2 along [101]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Primed axial glide planes</th>
<th>Two glide vectors: 1/2 along [100] and 1/2 along [011]</th>
<th>Two glide vectors: 1/2 along [010] and 1/2 along [101]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unprimed diamond</td>
<td>1/2 along</td>
<td>1/2 along</td>
</tr>
<tr>
<td>------------------</td>
<td>-----------</td>
<td>-----------</td>
</tr>
<tr>
<td>glide plane</td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
<tr>
<td></td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Primed diamond</th>
<th>1/2 along</th>
<th>1/2 along</th>
</tr>
</thead>
<tbody>
<tr>
<td>glide plane</td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
<tr>
<td></td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unprimed diamond</th>
<th>1/2 along</th>
<th>1/2 along</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
<tr>
<td></td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Primed diamond</th>
<th>1/2 along</th>
<th>1/2 along</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
<tr>
<td></td>
<td>[1{1}1]</td>
<td>[1{1}1]</td>
</tr>
</tbody>
</table>
2.2.3.7 Height of symmetry operations above plane of projection

Heights are given as a fraction of the shortest primed or unprimed translation perpendicular to the plane of projection. Fractions are color coded black and red corresponding to related unprimed and primed operations, respectively. Examples are as follows:

2.2.3.7a Rotation axes, screw axes, inversion axes and reflection and glide planes parallel to the plane of projection

2.2.3.7b Inversion centers and inversion axes perpendicular to the plane of projection (i.e. height of inversion center of rotation-inversion)
<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Graphical Symbol</th>
<th>Printed Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unprimed reflection line, mirror line</td>
<td>m</td>
<td>m</td>
</tr>
<tr>
<td>Primed reflection line, mirror line</td>
<td>m’</td>
<td>m’</td>
</tr>
<tr>
<td>Unprimed glide line, ½ lattice vector along line in plane</td>
<td>g</td>
<td>g</td>
</tr>
<tr>
<td>Primed glide line, ½ lattice vector along line in plane</td>
<td>g’</td>
<td>g’</td>
</tr>
<tr>
<td>Unprimed two-fold rotation point</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Primed two-fold rotation point</td>
<td>2’</td>
<td>2’</td>
</tr>
<tr>
<td>Unprimed three-fold rotation point</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Primed three-fold rotation point</td>
<td>3’</td>
<td>3’</td>
</tr>
<tr>
<td>Unprimed four-fold rotation point</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Primed four-fold rotation point</td>
<td>4’</td>
<td>4’</td>
</tr>
<tr>
<td>Unprimed six-fold rotation point</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Primed six-fold rotation point</td>
<td>6’</td>
<td>6’</td>
</tr>
</tbody>
</table>
Table 2.2.3-1D Graphical Symbols

One-Dimensional Magnetic Space Groups

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Graphical Symbol</th>
<th>Printed Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unprimed point of reflection</td>
<td>![Graphical Symbol]</td>
<td>m</td>
</tr>
<tr>
<td>Primed point of reflection</td>
<td>![Graphical Symbol]</td>
<td>m'</td>
</tr>
</tbody>
</table>
Table 3 - 1D:

One-Dimensional Magnetic Space Group Tables

ONE-DIMENSIONAL MAGNETIC SPACE GROUP INDEX

Figures 1.1-3D: Three-dimensional Magnetic Space Group Lattices
Figures 1.1-2D: Two-dimensional Magnetic Space Group Lattices
Index of One-Dimensional Magnetic Space Groups

1.1.1 \( p1 \)
1.2.2 \( p11' \)
1.3.3 \( p_{2a1} \)

2.1.4 \( pm \)
2.2.5 \( pm1' \)
2.3.6 \( pm' \)
2.4.7 \( p_{2a}m \)
Origin arbitrary

Asymmetric unit \(0 \leq z \leq 1\)

Symmetry operations

\((1) 1\)
\((1|0,0,0)\)

Generators selected \((1); \ t(1)\)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
</table>

| 1 a 1 | (1) x [u] |
Origin arbitrary

Asymmetric unit  \( 0 \leq x \leq 1 \)

Symmetry operations

For \(1+\) set
\[
(1)\ 1 \\
(1|0)
\]

For \(1'+\) set
\[
(1)\ 1' \\
(1|0)'
\]

Generators selected  (1); t(1); 1'

Positions

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>1+</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 a 11' (1) x [0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
$p_{2a1}$

No. 1.3.3

$p_{2a1}$

Origin arbitrary

Asymmetric unit  $0 \leq x \leq 1$

Symmetry operations

For $(0) +$ set

(1) 1
    (1\mid 0)

For $(1)' +$ set

(1) t' (1)
    (1\mid 1)'

Generators selected $(1); t(1)'$

Positions

Coordinates

Multiplicity,
Wyckoff letter,
Site symmetry

(0)+  (1)' +

1  a  1  (1) x [u]
Origin on mirror m

Asymmetric unit $0 \leq x \leq \frac{1}{2}$

Symmetry operations

(1) 1  (2) m 0
(1|0)  (m|0)

Generators selected (1); t(1); (2)

Positions

<table>
<thead>
<tr>
<th>Multiplicity,</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 c 1</td>
<td>(1) x [u]</td>
</tr>
<tr>
<td>1 b m</td>
<td>1/2 [u]</td>
</tr>
<tr>
<td>1 a m</td>
<td>0 [u]</td>
</tr>
</tbody>
</table>

TABLE 3 - 1D -4
TABLE 3 - 1D -5

Origin on mirror m1’

Asymmetric unit 0 ≤ x ≤ ½

Symmetry operations

For 1 + set
(1) 1 (2) m 0
    (1|0)        (m|0)

For 1’ + set
(1) 1’ (2) m’ 0
    (1|0)’        (m|0)’

Generators selected (1); t(1); (2); 1’

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 c 11’</td>
<td>(1) x [0]</td>
<td>(2) −x [0]</td>
<td></td>
</tr>
<tr>
<td>1 b m1’</td>
<td>1/2 [0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a m1’</td>
<td>0 [0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

TABLE 3 - 1D -5
**Origin** on mirror $m'$

**Asymmetric unit** $0 \leq x \leq \frac{1}{2}$

**Symmetry operations**

(1) $1$
(2) $m' \ 0$

(1|0) \quad (m|0)'

**Generators selected** (1); t(1); (2)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 c 1</td>
<td>(1) x [u]</td>
</tr>
<tr>
<td></td>
<td>(2) $\bar{x}$ [u]</td>
</tr>
<tr>
<td>1 b m'</td>
<td>1/2 [0]</td>
</tr>
<tr>
<td>1 a m'</td>
<td>0 [0]</td>
</tr>
</tbody>
</table>
### Table 3 - 1D -7

<table>
<thead>
<tr>
<th>No. 2.4.7</th>
<th>( p_{2a}m )</th>
<th>( m1' )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Origin</strong></td>
<td>on mirror ( m )</td>
<td></td>
</tr>
<tr>
<td><strong>Asymmetric unit</strong></td>
<td>( 0 \leq x \leq \frac{1}{2} )</td>
<td></td>
</tr>
</tbody>
</table>

#### Symmetry operations

For \((0) + \) set:

- \((1) \); \((2) m \) \(0\) \((m|0)\)
- \((1|0)\)

For \((1)' + \) set:

- \((1) t' (1) \); \((2) m' \) \(1/2\) \((m|1)'
- \((1|1)'

#### Generators selected

\((1); \ t(1)'; \ (2)\)

#### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>((0)+)</th>
<th>((1)' +)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2 \ c \ 1)</td>
<td>((1) x [u])</td>
<td>((2) \bar{x} [u])</td>
</tr>
<tr>
<td>(1 \ b \ m')</td>
<td>(1/2 [0])</td>
<td></td>
</tr>
<tr>
<td>(1 \ a \ m)</td>
<td>(0 [u])</td>
<td></td>
</tr>
</tbody>
</table>

*TABLE 3 - 1D -7*
Table 3 - 2D:

Two-Dimensional Magnetic Space Group Tables

TWO-DIMENSIONAL MAGNETIC SPACE GROUP INDEX

Table 3 - 3D: Three-Dimensional Magnetic Space Group Tables
Table 3 - 1D: One-Dimensional Magnetic Space Group Tables
<table>
<thead>
<tr>
<th>Index</th>
<th>Symbol</th>
<th>No. 1</th>
<th>No. 2</th>
<th>No. 3</th>
<th>No. 4</th>
<th>No. 5</th>
<th>No. 6</th>
<th>No. 7</th>
<th>No. 8</th>
<th>No. 9</th>
<th>No. 10</th>
<th>No. 11</th>
<th>No. 12</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1.1</td>
<td>p1</td>
<td>8.1.38 p2gg</td>
<td>17.1.76 p6mm</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.2.2</td>
<td>p11'</td>
<td>8.2.39 p2gg1'</td>
<td>17.2.77 p6mm1'</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.3.3</td>
<td>p2a1</td>
<td>8.3.40 p2g'g'</td>
<td>17.3.78 p6m'm'</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.1.4</td>
<td>p211</td>
<td>8.4.41 p2'gg'</td>
<td>17.4.79 p6'mm'</td>
<td></td>
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</table>
Origin arbitrary

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1$

Symmetry operations

(1) 1
    (1|0,0)
Continued

Generators selected  (1);  t(1,0);  t(0,1)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
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</thead>
<tbody>
<tr>
<td>1  a  1</td>
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<tr>
<td>(1) x,y [u,v]</td>
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Symmetry of special projections

<table>
<thead>
<tr>
<th>Along [10] p1</th>
<th>Along [01] p1</th>
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</thead>
<tbody>
<tr>
<td>a* = b_p</td>
<td>a* = a_p</td>
</tr>
<tr>
<td>Origin at x,0</td>
<td>Origin at 0,y</td>
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</tbody>
</table>
Origin arbitrary $1'$

Asymmetric unit $0 \leq x \leq 1; \ 0 \leq y \leq 1$

Symmetry operations

For $1 +$ set

(1) $1$

(1|0,0)

For $1' +$ set

(1) $1'$

(1|0,0)'
**Table 3 - 2D**

**Continued**

**No. 1.2.2**

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<th>(1); t(1,0); t(0,1); 1'</th>
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**Positions**

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<th>Coefficients</th>
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<td>1+ 1' +</td>
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<table>
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<tr>
<th>1 a 11'</th>
<th>(1) x,y</th>
<th>[0,0]</th>
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**Symmetry of special projections**

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<td>a* = b_p</td>
<td>a* = a_p</td>
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</table>

<table>
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<tr>
<th>Origin at x,0</th>
<th>Origin at 0,y</th>
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</thead>
</table>

**TABLE 3 - 2D -4**
Origin arbitrary

Asymmetric unit  \(0 \leq x \leq 1; \quad 0 \leq y \leq 1\)

Symmetry operations

For \((0,0)\) + set

\[
\begin{array}{l}
(1) 1 \\
(1|0,0)
\end{array}
\]

For \((1,0)\)' + set

\[
\begin{array}{l}
(1) t' (1,0) \\
(1|1,0)'
\end{array}
\]
Generators selected  (1);  t(1,0)';  t(0,1)

Positions

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

      (0,0)+  (1,0)' +

1  a  1  (1) x,y  [u,v]

Symmetry of special projections

Along [10] \( p11' \)    Along [01] \( p_{2a}' \)
\( a^* = b_p \)      \( a^* = a_p \)
Origin at x,0         Origin at 0,y
Origin on 2

Asymmetric unit  \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1 \)

Symmetry operations

(1) 1  \( (1|0,0) \)  \( (1|0,0) \)  \( (1|0,0) \)  \( (1|0,0) \)

(2) 2 0,0  \( (2|0,0) \)  \( (2|0,0) \)  \( (2|0,0) \)  \( (2|0,0) \)
Generators selected  (1): t(1,0); t(0,1);  (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry

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<th>Site symmetry</th>
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<tr>
<td>2 e 1</td>
<td>x,y [u,v]</td>
<td>(1) x,y [u,v]</td>
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<td>1 d 2</td>
<td>1/2,1/2 [0,0]</td>
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<td>1 c 2</td>
<td>1/2,0 [0,0]</td>
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<td>1 b 2</td>
<td>0,1/2 [0,0]</td>
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<td>0,0 [0,0]</td>
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Symmetry of special projections

Along [10] p1m'1  Along [01] p1m'1
a* = b_p  a* = a_p
Origin at x,0  Origin at 0,y

TABLE 3 - 2D -8
Origin on 21'  

Asymmetric unit  \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1 \)

Symmetry operations

For 1 + set

1

\((1|0,0)\)  

(2) \(2\ 0,0\)

\((2_z|0,0)\)

For 1' + set

1'

\((1|0,0)'\)

(2) \(2'\ 0,0\)

\((2_z|0,0)'\)
Generators selected
(1): t(1,0); t(0,1); (2): 1

Positions

Multiplicity, Wyckoff letter, Site symmetry

<table>
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<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 e 11'</td>
<td>(1) x,y [0,0]</td>
<td>(2) x̅,y̅ [0,0]</td>
</tr>
<tr>
<td>1 d 21'</td>
<td>1/2,1/2 [0,0]</td>
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<tr>
<td>1 c 21'</td>
<td>1/2,0 [0,0]</td>
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<tr>
<td>1 b 21'</td>
<td>0,1/2 [0,0]</td>
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<tr>
<td>1 a 21'</td>
<td>0,0 [0,0]</td>
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Symmetry of special projections

Along [10] pm 1'  Along [01] pm 1'

a* = b  a* = a  
Origin at x,0  Origin at 0,y
<table>
<thead>
<tr>
<th>Origin</th>
<th>Asymmetric unit</th>
<th>Symmetry operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>on 2'</td>
<td>$0 \leq x \leq 1/2$;</td>
<td>(1) 1</td>
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<td></td>
<td>$0 \leq y \leq 1$</td>
<td>(2) 2' 0,0</td>
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<td>(1</td>
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<td>(2</td>
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</tbody>
</table>
Generators selected  (1):  t(1,0);  t(0,1);  (2)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

\[
\begin{align*}
2 & \text{ e 1} \quad (1) \ x,y [u,v] \quad (2) \ \bar{x},\bar{y} [u,v] \\
1 & \text{ d 2'} \quad 1/2,1/2 [u,v] \\
1 & \text{ c 2'} \quad 1/2,0 [u,v] \\
1 & \text{ b 2'} \quad 0,1/2 [u,v] \\
1 & \text{ a 2'} \quad 0,0 [u,v] \\
\end{align*}
\]

Symmetry of special projections

Along [10] pm  Along [01] pm
\[a^* = b_p\]  \[a^* = a_p\]
Origin at x,0  Origin at 0,y
Origin on 2

Asymmetric unit  \( 0 \leq x \leq \frac{1}{2}; \ 0 \leq y \leq 1 \)

Symmetry operations

For \((0,0)\) + set

\[
\begin{align*}
(1) & \ 1 \\
(1) & \ (0,0) \\
(2) & \ 2 \ 0,0 \\
(2) & \ (2,0,0)
\end{align*}
\]

For \((1,0)\)' + set

\[
\begin{align*}
(1) & \ t' \ (1,0) \\
(1) & \ (1,0)' \\
(2) & \ 2' \ 1/2,0 \\
(2) & \ (2,1,0)'
\end{align*}
\]
Generators selected

(1): \(t(1,0)\); \(t(0,1)\); (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry

\[
\begin{align*}
(0,0) & + (1,0)' + \\
2 & e 1 \\
1 & d 2' \\
1 & c 2' \\
1 & b 2 \\
1 & a 2 \\
\end{align*}
\]

\[
\begin{align*}
(1) x,y [u,v] & \quad (2) \bar{x},\bar{y} [\bar{u},\bar{v}] \\
1/2,1/2 [u,v] & \quad 1/2,0 [u,v] \\
0,1/2 [0,0] & \quad 0,0 [0,0] \\
\end{align*}
\]

Symmetry of special projections

Along [10] \(p\overline{1}m1'\) Along [01] \(p_{2a}m'\)

\[
\begin{align*}
a^* &= b_p \\
a^* &= a_p \\
\end{align*}
\]

Origin at \(x,0\) Origin at \(0,y\)
**Origin** on mirror line \( m \)

**Asymmetric unit** \( 0 \leq x < 1/2; \quad 0 \leq y \leq 1 \)

**Symmetry operations**

\[
\begin{align*}
(1) & \quad 1 \\
(1|0,0) & \\
(2) & \quad m \quad 0, y \\
(m_\perp|0,0) & 
\end{align*}
\]
**Generators selected**  (1): t(1,0); t(0,1); (2)

**Positions**

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<td>1 b m</td>
<td>1/2,y [u,0]</td>
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<td>1 a m</td>
<td>0,y [u,0]</td>
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**Symmetry of special projections**

- Along [10] \( p11' \)
- Along [01] \( pm \)

\( a^* = b \)  
\( a^* = a \)  

Origin at x,0  
Origin at 0,y
Origin on mirror line $m_1'$

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1$

Symmetry operations

For $1 +$ set

(1) 1
(1) 0,0
(1) 0,0

(2) $m$ 0,0
(2) $m_{x}$ 0,0

For $1' +$ set

(1) 1'
(1) 0,0'
(1) 0,0'

(2) $m'$ 0,0
(2) $m_{x}$ 0,0

TABLE 3 - 2D -17
Generators selected

(1): t(1,0); t(0,1); (2): 1'

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>1' +</td>
</tr>
<tr>
<td>2 c 11'</td>
<td>(1) x,y [0,0] (2) \bar{x},y [0,0]</td>
</tr>
<tr>
<td>1 b m1'</td>
<td>1/2,y [0,0]</td>
</tr>
<tr>
<td>1 a m1'</td>
<td>0,y [0,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] p11' Along [01] pm1'

a* = b a* = a

Origin at x,0 Origin at 0,y
Origin on mirror line m'

Asymmetric unit  $0 \leq x \leq 1/2; \ 0 \leq y \leq 1$

Symmetry operations

(1) 1  \hspace{1cm} (2) $m' \ 0, y$

$(1 \ |0,0) \hspace{1cm} (m_x |0,0)'$
Continued No. 3.3.10 p1m'1

**Generators selected**
(1): t(1,0); t(0,1); (2)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 c 1</td>
<td>(1) x, y [u, v]</td>
</tr>
<tr>
<td></td>
<td>(2) x', y [u', v]</td>
</tr>
<tr>
<td>1 b m'</td>
<td>1/2, y [0, v]</td>
</tr>
<tr>
<td>1 a m'</td>
<td>0, y [0, v]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th>Along [10] p1</th>
<th>Along [01] pm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>a* = a</td>
</tr>
<tr>
<td>Origin at x, 0</td>
<td>Origin at 0, y</td>
</tr>
</tbody>
</table>

---

**TABLE 3 - 2D -20**
Origin on mirror line $m$

**Asymmetric unit** \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1 \)

**Symmetry operations**

For \((0,0) + \) set

1. \((1,0)\)
2. \(m\ 0, y\)
3. \((m_1,0)\)

For \((1,0)' + \) set

1. \((1,0)'\)
2. \(m' 1/2, y\)
3. \((m_1,1,0)'\)

**TABLE 3 - 2D -21**
Generators selected  (1);  t(1,0)';  t(0,1);  (2)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)+</td>
<td>(1,0)' +</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) x̅,y [u,ν]</td>
<td></td>
</tr>
<tr>
<td>1 b m'</td>
<td>1/2,y [0,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a m</td>
<td>0,y [u,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] p11'    Along [01] p_{2a}m
a* = b            a* = a
Origin at x,0     Origin at 0,y

TABLE 3 - 2D -22
TABLE 3 - 2D -23

 Origin on mirror line m

 Asymmetric unit  \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1 \)

 Symmetry operations

 For \((0,0)\) + set

 (1) 1  
 (2) m \(0,y\)  
 (1|0,0) \(m_x|0,0\)

 For \((0,1)\)' + set

 (1) \(t'\) \((0,1)\)  
 (2) \(g'\) \((0,1)\) \(0,y\)  
 (1|0,1)’ \((m_x|0,1)\)’
Generators selected  (1):  t(1,0);  t(0,1)';  (2)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)+</td>
</tr>
<tr>
<td>(0,1)' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2  c  1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)  x,y [u,v]</td>
</tr>
<tr>
<td>(2)  x̅,y [u,ν]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1  b  m</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2,y [u,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1  a  m</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,y [u,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] p11'  Along [01] pm1'

a* = b  a* = a

Origin at x,0  Origin at 0,y
Origin on mirror line $m'$

Asymmetric unit  $0 \leq x \leq 1/2; \hspace{1em} 0 \leq y \leq 1$

Symmetry operations

For $(0,0)$ set

(1) $1$  \hspace{1em} (2) $m' \hspace{1em} 0, y$

$(1|0,0) \hspace{1em} (m_x|0,0)'$

For $(0,1)'$ set

(1) $t' \hspace{1em} (0,1)$  \hspace{1em} (2) $g \hspace{1em} (0,1) \hspace{1em} 0, y$

$(1|0,1)' \hspace{1em} (m_x|0,1)$
Generators selected \( (1): t(1,0); t(0,1)^\prime; (2) \)

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0)^+)</td>
<td>((0,1)^\prime +)</td>
</tr>
<tr>
<td>(2 c 1)</td>
<td>((1) x,y [u,v]) (2) \bar{x},y [\bar{u},v])</td>
</tr>
<tr>
<td>(1 b m')</td>
<td>(1/2,y [0,v])</td>
</tr>
<tr>
<td>(1 a m')</td>
<td>(0,y [0,v])</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] \( p_{2a^*1} \) Along [01] \( p_{m1} \)
\( a^* = b \) \( a^* = a \)
Origin at x,0 Origin at 0,y
Origin on mirror line m

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1$

Symmetry operations

For $(0,0)$ set

1. $1$
2. $m \quad 0,y$

For $(0,1)'$ set

1. $t' \quad (0,1)$
2. $g' \quad (0,1) \quad 0,y$

$\begin{array}{c}
(1|0,0) \\
(m_x|0,0) \\
(1|0,1)' \\
(m_x|0,1)'
\end{array}$
**Generators selected**  
(1): t(1,0)' ; t(0,1)' ; (2)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0)+</td>
</tr>
<tr>
<td>2 c 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td>1 b m'</td>
<td>1/2, y [0,v]</td>
</tr>
<tr>
<td>1 a m</td>
<td>0, y [u,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**  
Along [1 0] p11'    
\[ a^* = b \]      
Origin at x,0  
Along [0 1] pm1'   
\[ a^* = a \]      
Origin at 0, y
Origin on glide line g

Asymmetric unit \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1 \)

Symmetry operations

\[
\begin{align*}
(1) \ 1 \\
(1|0,0) \\

(2) \ g \ (0,1/2) \ 0,y \\
(m,0,1/2)
\end{align*}
\]
Generators selected (1): \( t(1,0); \ t(0,1); \ (2) \)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site symmetry</td>
<td></td>
</tr>
<tr>
<td>2 ( a ) 1</td>
<td>(1) ( x,y \ [u,v] ) (2) ( x, y+1/2 \ [u,v] )</td>
</tr>
</tbody>
</table>

Symmetry of special projections

<table>
<thead>
<tr>
<th>Along [10] ( \text{p}_{2a} ) 11</th>
<th>Along [01] ( \text{p} ) m</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = b/2 )</td>
<td>( a^* = a )</td>
</tr>
<tr>
<td>Origin at ( x,0 )</td>
<td>Origin at ( 0,y )</td>
</tr>
</tbody>
</table>
**Origin** on glide line $g_1'$

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1$

**Symmetry operations**

For $1 +$ set

(1) $1$
(1) $0, 0$

(2) $g$  
(2) $(0, 1/2)$  
(2) $0, y$
(2) $(m_x, 0, 1/2)$

For $1' +$ set

(1) $1'$
(1) $(0, 0)'$

(2) $g'$  
(2) $(0, 1/2)$  
(2) $0, y$
(2) $(m_x, 0, 1/2)'$
Generators selected  (1): t(1,0); t(0,1); (2): 1'

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+ 1'</td>
<td>2 a 11'</td>
</tr>
<tr>
<td>11' (1) x,y [0,0]</td>
<td>(1) x,y [0,0]</td>
</tr>
<tr>
<td>1' (2) x̅,y+ 1/2 [0,0]</td>
<td>(2) x̅,y+ 1/2 [0,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] p1 1'  Along [01] pm 1'  
\( a^* = \frac{b}{2} \)  \( a^* = a \)
Origin at x,0  Origin at 0,y
Origin on glide line $g'$

Asymmetric unit: $0 \leq x \leq 1/2; \ 0 \leq y \leq 1$

Symmetry operations

(1) 1
(1|0,0)

(2) $g'$ (0,1/2) 0,x
(m|0,1/2)'
**Generators selected** (1); t(1,0); t(0,1); (2)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 a 1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x, y [u, v]</td>
</tr>
<tr>
<td>(2) ( \bar{x}, y + 1/2 ) [( \bar{u}, v )]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th>Along [10] p1</th>
<th>Along [01] pm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = b/2 )</td>
<td>( a^* = a )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Origin at x,0</th>
<th>Origin at 0, y</th>
</tr>
</thead>
</table>
Origin: on glide line g

Asymmetric unit: $0 \leq x \leq 1/2; \ 0 \leq y \leq 1$

Symmetry operations:

For $(0,0)$:

- $1$
- $g\ (0.1/2)\ 0,y$
- $(1|0,0)$
- $(m_x|0.1/2)$

For $(1,0)’$:

- $t’\ (1,0)$
- $g’\ (0.1/2)\ 1/2,y$
- $(1|1,0)'$
- $(m_x|1.1/2)'$
Generators selected

\begin{align*}
&1; \ t(1,0)^1; \ t(0,1); \ (2) \\
\end{align*}

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)+   \quad (1,0)' +</td>
</tr>
</tbody>
</table>

\begin{align*}
2 & a \ 1 \quad (1) \ x,y \ [u,v] \quad & (2) \ \bar{x},y+1/2 \ [u,\bar{v}] \\
\end{align*}

Symmetry of special projections

\begin{align*}
\text{Along [10]} & \quad p11' \quad \text{Along [01]} & \quad p_{2a^*m} \\
a^* = b/2 & \quad a^* = a \\
\text{Origin at } x,0 & \quad \text{Origin at } 0,y \\
\end{align*}
Origin on mirror line m

Asymmetric unit \( 0 \leq x \leq 1/4; \ 0 \leq y \leq 1 \)

Symmetry operations

For \((0,0) + \) set

(1) \( t \) \( (1/2,1/2) \)  
(1\( |\)0,0)  

(2) \( m \) \( 0,y \)  
(1\( |\)0,0)  

\( (m_1,0,0) \)

For \((1/2,1/2) + \) set

(1) \( t \) \( (1/2,1/2) \)  
(1\( |\)1/2,1/2)  

(2) \( g \) \( (0,1/2) \) \( 1/4,y \)  
(1\( |\)1/2,1/2)  

\( (m_1,1/2,1/2) \)
Continued

| No. 5.1.19 | c1m1 |

**Generators selected**

(1); t(1,0); t(0,1); t(1/2,1/2); (2)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) + (1/2,1/2) +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4 b 1</th>
<th>(1) x,y [u,v]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 a m</td>
<td>0,y [u,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] p11'    Along [01] pm

a* = b/2       a* = a/2

Origin at x,0     Origin at 0,y
| No. 5.2.20 | c1m11' | m1' |

**Origin** on mirror line m1'

**Asymmetric unit**  \(0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq 1\)

**Symmetry operations**

For \((0,0)\) + set

1. \(I\)  
2. \(m\) \((0,0)\)  
   \((m,0,0)\)

For \((1/2,1/2)\) + set

1. \(t\) \((1/2,1/2)\)  
2. \(g\) \((0,1/2)\) \(1/4, y\)
   \((m,1/2,1/2)\)

For \((0,0)\)' + set

1. \(I'\) \((0,0)\)'  
2. \(m'\) \((0,0)\)'  
   \((m,0,0)\)'

For \((1/2,1/2)\)' + set

1. \(t'\) \((1/2,1/2)\)'  
2. \(g'\) \((0,1/2)\) \(1/4, y\)
   \((m,1/2,1/2)\)'

**TABLE 3 - 2D -39**
Continued No. 5.2.20 c1m11'

Generators selected (1); t(1,0); t(0,1); t(1/2,1/2); (2); 1'

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) +</td>
</tr>
<tr>
<td>(1/2,1/2) +</td>
</tr>
<tr>
<td>(0,0)' +</td>
</tr>
<tr>
<td>(1/2,1/2)' +</td>
</tr>
</tbody>
</table>

Coordinates

| 4 b 11' (1) x,y [0,0] (2) x̅,y [0,0] |

| 2 a m1' 0,y [0,0] |

Symmetry of special projections

Along [10] p11' Along [01] pm1'

$\mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{a}^* = \mathbf{a}/2$

Origin at x,0 Origin at 0,y
Origin on mirror line m'

Asymmetric unit  \( 0 \leq x \leq 1/4; \, 0 \leq y \leq 1 \)

Symmetry operations

For (0,0) + set

(1) \(t\)  \((0,0)\)
(2) \(m'\)  \(0,y\)

\((1|0,0)\)  \((m_x|0,0)'\)

For (1/2,1/2) + set

(1) \(t\)  \((1/2,1/2)\)
(2) \(g'\)  \((0,1/2)\)

\((1|1/2,1/2)\)  \((m_x|1/2,1/2)'\)
Continued

No. 5.3.21  

Generators selected  
(1);  \(t(1,0);\)  \(t(0,1);\)  \(t(1/2,1/2);\)  (2)

Positions

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) + (1/2,1/2) +</td>
<td>4 b 1  ((1) x,y [u,v])  ((2) \bar{x}, y [\bar{u},v])</td>
</tr>
<tr>
<td>2 a m'</td>
<td>0,y [0,v]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] \(p1\)  
\(a^* = b/2\)  
Origin at \(x,0\)

Along [01] \(pm'\)  
\(a^* = a/2\)  
Origin at 0,\(y\)
### Origin

Origin on mirror line m

### Asymmetric unit

$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1$

### Symmetry operations

For $(0,0) +$ set

1. $1$
2. $m \quad 0,y$

For $(1/2,1/2)' +$ set

1. $t' \quad (1/2,1/2)$
2. $g' \quad (0,1/2) \quad 1/4,y$

TABLE 3 - 2D -43
Generators selected

(1); t(1,0); t(0,1); t(1/2,1/2)'; (2)

Positions

Coordinates

Multiplicity,
Wyckoff letter,
Site symmetry

(0,0) +
(1/2,1/2)' +

4 b 1 (1) x,y [u,v] (2) x̅,y [u,ν]

2 a m 0,y [u,0]

Symmetry of special projections

Along [10] p11'  Along [01] p2a'm

a* = b/2  a* = a/2

Origin at x,0  Origin at 0,y
TABLE 3 - 2D - 45

No. 5. 5. 23

 Origin on mirror line m'

Asymmetric unit  \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1\)

Symmetry operations

For \((0,0) +\) set

\[
\begin{align*}
(1) & \quad 1 \\
(1 | 0,0) & \quad (m | 0,0)'
\end{align*}
\]

For \((1/2,1/2)' +\) set

\[
\begin{align*}
(1)' & \quad (1/2,1/2) \\
(1 | 1/2,1/2)' & \quad (m_s|1/2,1/2)
\end{align*}
\]

\[
\begin{align*}
(1) & \quad (1/2,1/2) \\
(1 | 0,1/2) & \quad 1/4, y
\end{align*}
\]
Generators selected
(1): t(1,0); t(0,1); t(1/2,1/2)'; (2)

Positions
Coordinates

Multiplicity,
Wyckoff letter,
Site symmetry

(0,0) + (1/2,1/2)'

4 b 1 (1) x,y [u,v] (2) x̅,y [u̅,v]

2 a m' 0,y [0,v]

Symmetry of special projections
Along [10] \( p_{2a} \) Along [01] \( p_{2a} \) m
\( a^* = b/2 \) \( a^* = a/2 \)
Origin at x,0 Origin at 1/4,y
**Origin** on 2mm

**Asymmetric unit**  \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2 \)

**Symmetry operations**

1. \( 1 \)  
   \( (1;0,0) \)
2. \( 2 \)  
   \( (2_x;0,0) \)
3. \( m \)  
   \( (m_y;0,0) \)
4. \( m \)  
   \( (m_x;0,0) \)
**Generators selected**  (1): t(1,0); t(0,1); (2): (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>(1) x, y [u, v] (2) ( \bar{x}, \bar{y} [u, v] ) (3) x, ( \bar{y} [u, v] ) (4) ( \bar{x}, y [u, v] )</td>
</tr>
<tr>
<td>2 h .m.</td>
<td>1/2, y [u, 0] 1/2, ( \bar{y} [u, 0] )</td>
</tr>
<tr>
<td>2 g .m.</td>
<td>0, y [u, 0] 0, ( \bar{y} [u, 0] )</td>
</tr>
<tr>
<td>2 f ..m</td>
<td>x, 1/2 [0, v] ( \bar{x}, 1/2 [0, v] )</td>
</tr>
<tr>
<td>2 e ..m</td>
<td>x, 0 [0, v] ( \bar{x}, 0 [0, v] )</td>
</tr>
<tr>
<td>1 d 2mm</td>
<td>1/2, 1/2 [0, 0]</td>
</tr>
<tr>
<td>1 c 2mm</td>
<td>1/2, 0 [0, 0]</td>
</tr>
<tr>
<td>1 b 2mm</td>
<td>0, 1/2 [0, 0]</td>
</tr>
<tr>
<td>1 a 2mm</td>
<td>0, 0 [0, 0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] \( pm1' \) \( a^* = b \) Origin at x,0
- Along [01] \( pm1' \) \( a^* = a \) Origin at 0, y

---

**TABLE 3 - 2D -48**
**Origin** on 2mm1'

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2$

**Symmetry operations**

For 1 + set

1. $1$  
   $(1|0,0)$

2. $2$  
   $(2z|0,0)$

3. $m$  
   $(m_y|0,0)$

4. $m$  
   $(m_z|0,0)$

For 1' + set

1. $1'$  
   $(1|0,0)'$

2. $2'$  
   $(2z|0,0)'$

3. $m'$  
   $(m_y|0,0)'$

4. $m'$  
   $(m_z|0,0)'$
**Generators selected**  (1);  t(1,0);  t(0,1);  (2);  (3);  1’

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site symmetry</td>
<td>1+  1’  +</td>
</tr>
<tr>
<td>4 i 11’</td>
<td>(1) x,y [0,0]   (2) x̅,y [0,0]   (3) x̅,y [0,0]   (4) x̅,y [0,0]</td>
</tr>
<tr>
<td>2 h .m.1’</td>
<td>1/2,y [0,0]   1/2,y [0,0]</td>
</tr>
<tr>
<td>2 g .m.1’</td>
<td>0,y [0,0]   0,y [0,0]</td>
</tr>
<tr>
<td>2 f ..m1’</td>
<td>x,1/2 [0,0]   x̅,1/2 [0,0]</td>
</tr>
<tr>
<td>2 e ..m1’</td>
<td>x,0 [0,0]   x̅,0 [0,0]</td>
</tr>
<tr>
<td>1 d 2mm1’</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>1 c 2mm1’</td>
<td>1/2,0 [0,0]</td>
</tr>
<tr>
<td>1 b 2mm1’</td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td>1 a 2mm1’</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th>Along [10] pm1’</th>
<th>Along [01] pm1’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>a* = a</td>
</tr>
<tr>
<td>Origin at x,0</td>
<td>Origin at 0,y</td>
</tr>
</tbody>
</table>

TABLE 3 - 2D -50
**Origin** on $2m'm'$

**Asymmetric unit** $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2$

**Symmetry operations**

1. $1$  \hspace{1cm} (1) $1$
   \hspace{1cm} (1:0,0)
2. $2 \ 0,0$  \hspace{1cm} (2) $2 \ 0,0$
   \hspace{1cm} (2:0,0)
3. $m' \ x,0$  \hspace{1cm} (3) $m' \ x,0$
   \hspace{1cm} (m:0,0')
4. $m' \ 0,y$  \hspace{1cm} (4) $m' \ 0,y$
   \hspace{1cm} (m:0,0')

**TABLE 3 - 2D -51**
Generators selected \( (1); \ t(1,0); \ t(0,1); \ (2); \ (3) \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity,</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wyckoff letter,</td>
<td>Site symmetry</td>
</tr>
<tr>
<td>Symmetry of special projections</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4\ i\ 1)</td>
<td>(1)</td>
<td>(x, y [u, v])</td>
</tr>
<tr>
<td></td>
<td>(2)</td>
<td>(\bar{x}, \bar{y} [\bar{u}, \bar{v}])</td>
</tr>
<tr>
<td></td>
<td>(3)</td>
<td>(x, \bar{y} [u, \bar{v}])</td>
</tr>
<tr>
<td></td>
<td>(4)</td>
<td>(\bar{x}, y [\bar{u}, v])</td>
</tr>
<tr>
<td>(2\ h\ .m'.)</td>
<td>(1/2, y [0, v])</td>
<td>(1/2, \bar{y} [0, \bar{v}])</td>
</tr>
<tr>
<td>(2\ g\ .m'.)</td>
<td>(0, y [0, v])</td>
<td>(0, \bar{y} [0, \bar{v}])</td>
</tr>
<tr>
<td>(2\ f\ .m')</td>
<td>(x, 1/2 [u, 0])</td>
<td>(\bar{x}, 1/2 [\bar{u}, 0])</td>
</tr>
<tr>
<td>(2\ e\ .m')</td>
<td>(x, 0 [u, 0])</td>
<td>(\bar{x}, 0 [\bar{u}, 0])</td>
</tr>
<tr>
<td>(1\ d\ 2m'm')</td>
<td>(1/2, 1/2 [0, 0])</td>
<td></td>
</tr>
<tr>
<td>(1\ c\ 2m'm')</td>
<td>(1/2, 0 [0, 0])</td>
<td></td>
</tr>
<tr>
<td>(1\ b\ 2m'm')</td>
<td>(0, 1/2 [0, 0])</td>
<td></td>
</tr>
<tr>
<td>(1\ a\ m'm'2)</td>
<td>(0, 0 [0, 0])</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th>Along [10] pm'</th>
<th>Along [01] pm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = b)</td>
<td>(a^* = a)</td>
</tr>
<tr>
<td>Origin at (x, 0)</td>
<td>Origin at (0, y)</td>
</tr>
</tbody>
</table>
Origin on 2'\text{mm}''

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2 \)

Symmetry operations

\begin{align*}
(1) & \quad 1 \quad (2) & \quad 2' \quad 0,0 \\
& \quad (1;0,0) \quad & \quad (2_z;0,0)' \\
(3) & \quad m' \quad x,0 \\
& \quad (m;0,0)' \\
(4) & \quad m \quad 0,y \\
& \quad (m_x;0,0)' 
\end{align*}
Generators selected \((1); \ t(1,0); \ t(0,1); \ (2); \ (3)\)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>((1) \ x,y \ [u,v])</td>
</tr>
<tr>
<td></td>
<td>((3) \ x, \bar{y} \ [u,\bar{v}])</td>
</tr>
<tr>
<td>2 h .m.</td>
<td>(1/2, y \ [u,0])</td>
</tr>
<tr>
<td>2 g .m.</td>
<td>(0, y \ [u,0])</td>
</tr>
<tr>
<td>2 f .m’</td>
<td>(x, 1/2 \ [u,0])</td>
</tr>
<tr>
<td>2 e .m’</td>
<td>(x, 0 \ [u,0])</td>
</tr>
<tr>
<td>1 d 2’mm’</td>
<td>(1/2, 1/2 \ [u,0])</td>
</tr>
<tr>
<td>1 c 2’mm’</td>
<td>(1/2, 0 \ [u,0])</td>
</tr>
<tr>
<td>1 b 2’mm’</td>
<td>(0, 1/2 \ [u,0])</td>
</tr>
<tr>
<td>1 a 2’mm’</td>
<td>(0, 0 \ [u,0])</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] pm1’\(\ qm\)Along [01] pm\(\ qm\)

\(a^* = b\) \(a^* = a\)

Origin at \(x,0\) Origin at \(0,y\)

---

**TABLE 3 - 2D -54**
**Origin** on 2m\'m'  

**Asymmetric unit**  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2 \]

**Symmetry operations**

For (0,0) + set

1. 1
2. 2 0,0
   (1) (0,0)  
   (2) (2,0)
3. m' x,0
   (1) m' 0,0'  
   (2) (m,0)
4. m' 0,y
   (1) m' 0,0'  
   (2) (m,0)

For (1,0)' + set

1. t' (1,0)
2. 2' 1/2,0
   (1) (1,0)'  
   (2) (2,1,0)' 
3. g (1,0) x,0
   (1) g (1,0)'  
   (2) (g,1,0)
4. m 1/2,y
   (1) (m,1)' 
   (2) (m,1)
### Generators selected

(1) \( t(1.0)' \); \( t(0.1) \); (2); (3)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)+</td>
<td>(1,0)' +</td>
</tr>
<tr>
<td>4 i 1</td>
<td>(1) ( x,y ) [u,v]</td>
</tr>
<tr>
<td></td>
<td>(3) ( x, \bar{y} ) [u,( v )]</td>
</tr>
<tr>
<td>2 h .m.</td>
<td>1/2,( y ) [u,0]</td>
</tr>
<tr>
<td>2 g .m'.</td>
<td>0,( y ) [0,( v )]</td>
</tr>
<tr>
<td>2 f .m'</td>
<td>( x,1/2 ) [u,0]</td>
</tr>
<tr>
<td>2 e .m'</td>
<td>( x,0 ) [u,0]</td>
</tr>
<tr>
<td>1 d 2'mm'</td>
<td>1/2,1/2 [u,0]</td>
</tr>
<tr>
<td>1 c 2'mm'</td>
<td>1/2,0 [u,0]</td>
</tr>
<tr>
<td>1 b 2'm'm'</td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td>1 a 2'm'm'</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- **Along [10] pm1'**
  - \( a^* = b \)
  - Origin at \( x,0 \)
- **Along [01] \( p_{2a}m \)**
  - \( a^* = a \)
  - Origin at \( 1/2,y \)

---

**TABLE 3 - 2D -56**
Origin on 2mm

Asymmetric unit  $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2$

Symmetry operations

For (0,0) + set

1. $I (1,0,0)$
2. $2 (2,0,0)$
3. $m x,0 (m_x,0,0)$
4. $m 0,y (m_x,0,0)$

For (0,1) + set

1. $t' (0,1,0,1)$
2. $2' (0,1/2,0,1)$
3. $m' x,1/2 (m_x,0,1)$
4. $g' (0,1,0,1)$

TABLE 3 - 2D -57
**Generators selected**  (1);  t(1,0)';  t(0,1)';  (2);  (3)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) (\bar{x},y [\bar{u},v])</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) (x,\bar{y} [\bar{u},v])</td>
<td>(4) (\bar{x},y [u,\bar{v}])</td>
<td></td>
</tr>
<tr>
<td>2 h .m'</td>
<td>1/2,y [0,v]</td>
<td>1/2,(\bar{y} [0,v])</td>
<td></td>
</tr>
<tr>
<td>2 g .m</td>
<td>0,y [u,0]</td>
<td>0,(\bar{y} [\bar{u},0])</td>
<td></td>
</tr>
<tr>
<td>2 f .m'</td>
<td>x,1/2 [u,0]</td>
<td>(\bar{x},1/2 [u,0])</td>
<td></td>
</tr>
<tr>
<td>2 e .m</td>
<td>x,0 [0,v]</td>
<td>(\bar{x},0 [0,\bar{v}])</td>
<td></td>
</tr>
<tr>
<td>1 d 2m'm'</td>
<td>1/2,1/2 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 c 2'm'm'</td>
<td>1/2,0 [0,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 b 2'm'm'</td>
<td>0,1/2 [u,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a 2mm</td>
<td>0,0 [0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- Along [10] \(p1m'\)  
  - \(a'^* = b\)
  - Origin at \(x,0\)

- Along [01] \(p1m'\)  
  - \(a'^* = a\)
  - Origin at \(0,y\)
### Origin
Origin on 2mm

### Asymmetric unit
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2$

### Symmetry operations

<table>
<thead>
<tr>
<th>For (0,0) + set</th>
<th>(1) 1 (1,0)</th>
<th>(2) 2 2,0 (2,0)</th>
<th>(3) m x,0 (m,0)</th>
<th>(4) m 0,y (m,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1 (0,0)</td>
<td>(2) 2 0,0 (2,0)</td>
<td>(3) m x,0 (m,0)</td>
<td>(4) m 0,y (m,0)</td>
<td></td>
</tr>
<tr>
<td>For (1,0)' + set</td>
<td>(1) t' (1,0)</td>
<td>(2) 2' 1/2,0 (2,0)'</td>
<td>(3) g' (1,0) x,0 (m,0)'</td>
<td>(4) m' 1/2,y (m,0)'</td>
</tr>
<tr>
<td>(1) 1</td>
<td>(2) 2 (2,0)</td>
<td>(3) m x,0 (m,0)</td>
<td>(4) m 0,y (m,0)</td>
<td>(m,0)'</td>
</tr>
<tr>
<td>(1,0)'</td>
<td>(2,0)'</td>
<td>(m,0)'</td>
<td>(m,0)'</td>
<td>(m,0)'</td>
</tr>
</tbody>
</table>
Generators selected (1); t(1,0)'; t(0,1); (2); (3)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) (\bar{x},\bar{y} [u,v])</td>
</tr>
<tr>
<td></td>
<td>(3) x,(\bar{y}) [(\bar{u},v)]</td>
<td>(4) (\bar{x},y [u,\bar{v}])</td>
</tr>
<tr>
<td>2 h .m'</td>
<td>1/2,y [0,v]</td>
<td>1/2,(\bar{y}) [0,v]</td>
</tr>
<tr>
<td>2 g .m</td>
<td>0,y [u,0]</td>
<td>0,(\bar{y}) [(\bar{u},0)]</td>
</tr>
<tr>
<td>2 f ..m</td>
<td>x,1/2 [0,v]</td>
<td>(\bar{x},1/2 [0,\bar{v}])</td>
</tr>
<tr>
<td>2 e ..m</td>
<td>x,0 [0,v]</td>
<td>(\bar{x},0 [0,\bar{v}])</td>
</tr>
<tr>
<td>1 d 2'm'm</td>
<td>1/2,1/2 [0,v]</td>
<td></td>
</tr>
<tr>
<td>1 c 2'm'm</td>
<td>1/2,0 [0,v]</td>
<td></td>
</tr>
<tr>
<td>1 b 2mm</td>
<td>0,1/2 [0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a 2mm</td>
<td>0,0 [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] \(p1m11'\)    Along [01] \(p1m11'\)
\(a^* = b\)               \(a^* = a\)
Origin at x,0,0            Origin at 0,y,0
Origin on 21g

Asymmetric unit  \( 0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq 1 \)

Symmetry operations

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(1;0,0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2)</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>(2;0,0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3)</td>
<td>g</td>
<td>(1/2,0)</td>
<td>x</td>
</tr>
<tr>
<td></td>
<td>(m;1/2,0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4)</td>
<td>m</td>
<td>1/4</td>
<td>y</td>
</tr>
<tr>
<td></td>
<td>(m;1/2,0)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Generators selected
(1); t(1,0); t(0,1); (2); (3)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,\̅y [u\̅,v]</td>
</tr>
<tr>
<td>2 c .m.</td>
<td>1/4,y [u,0]</td>
</tr>
<tr>
<td>2 b 2..</td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td>2 a 2..</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- Along [10] pm1':
  - \(a^* = b\)
  - Origin at x,0

- Along [01] \(p_{2a}\cdot m\):
  - \(a^* = a/2\)
  - Origin at 1/4,y
Origin on 21g1'

Asymmetric unit  \( 0 \leq x \leq 1/4; \ 0 \leq y \leq 1 \)

Symmetry operations

For 1 + set

(1) 1  
\((1|0,0)\)

(2) 2 0,0  
\((2_2|0,0)\)

(3) \(g\)  \((1/2,0)\)  \(x,0\)  
\((m_y|1/2,0)\)

(4) \(m\)  \(1/4,y\)  
\((m_x|1/2,0)\)

For 1' + set

(1) 1'  
\((1|0,0)\)'

(2) 2' 0,0  
\((2_2|0,0)\)'

(3) \(g'\)  \((1/2,0)\)  \(x,0\)  
\((m_y|1/2,0)'\)

(4) \(m'\)  \(1/4,y\)  
\((m_x|1/2,0)'\)
**Generators selected**  
(1); t(1,0); t(0,1); (2); (3); 1’

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site symmetry</td>
<td>1+ 1’ +</td>
</tr>
<tr>
<td>4 d 11’</td>
<td>(1) x, y [0,0] (2) x, y [0,0] (3) x+1/2, y [0,0] (4) x+1/2, y [0,0]</td>
</tr>
<tr>
<td>2 c .m.1’</td>
<td>1/4, y [0,0] 3/4, y [0,0]</td>
</tr>
<tr>
<td>2 b 2..1’</td>
<td>0, 1/2 [0,0] 1/2, 1/2 [0,0]</td>
</tr>
<tr>
<td>2 a 2..1’</td>
<td>0, 0 [0,0] 1/2, 0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th>Along [10] pm 1’</th>
<th>Along [01] pm 1’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>a* = a/2</td>
</tr>
<tr>
<td>Origin at x, 0</td>
<td>Origin at 0, y</td>
</tr>
</tbody>
</table>
Origin on 21g'

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1

Symmetry operations

1. 1
2. 2 0,0
3. g' (1/2,0) x,0
4. m' 1/4,y

TABLE 3 - 2D -65
Generators selected  (1);  t(1,0);  t(0,1);  (2);  (3)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site symmetry</td>
<td></td>
</tr>
<tr>
<td>4  d  1</td>
<td>(1) x,y [u,v]  (2) x,y [u,v]  (3) x+1/2,y [u,v]  (4) x+1/2,y [u,v]</td>
</tr>
<tr>
<td>2  c  .m'</td>
<td>1/4,y [u,v]  3/4,y [0,v]</td>
</tr>
<tr>
<td>2  b  2..</td>
<td>0,1/2 [0,0]  1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>2  a  2..</td>
<td>0,0 [0,0]  1/2,0 [0,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] pm'  Along [01] pm'
\( a^* = b \)  \( a^* = a/2 \)
Origin at x,0  Origin at 0,y
### Table 3 - 2D - 67

<table>
<thead>
<tr>
<th>Symmetry Operations</th>
<th>p2'm'g</th>
<th>2'm'm</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Origin</strong></td>
<td>on 2'1g</td>
<td></td>
</tr>
<tr>
<td><strong>Asymmetric unit</strong></td>
<td>[0 \leq x \leq 1/4; 0 \leq y \leq 1]</td>
<td></td>
</tr>
<tr>
<td><strong>Symmetry operations</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(1) 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(1</td>
<td>0,0)</td>
<td></td>
</tr>
<tr>
<td>(2) 2' 0,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2_2</td>
<td>0,0)'</td>
<td></td>
</tr>
<tr>
<td>(3) g (1/2,0) x,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(m_1</td>
<td>1/2,0)</td>
<td></td>
</tr>
<tr>
<td>(4) m' 1/4,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(m_x</td>
<td>1/2,0)'</td>
<td></td>
</tr>
</tbody>
</table>
**Generators selected**  (1); t(1,0); t(0,1); (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 4 d 1        | (1) x,y [u,v]  
              | (2) x, y [u,v] |
|              | (3) x+1/2, y [u,v]  
              | (4) x+1/2, y [u,v] |
| 2 c .m'      | 1/4, y [0,v]  
              | 3/4, y [0,v] |
| 2 b 2'..     | 0,1/2 [u,v]  
              | 1/2,1/2 [u,v] |
| 2 a 2'..     | 0,0 [u,v]  
              | 1/2,0 [u,v] |

**Symmetry of special projections**

Along [10] \( \rho m \)  
Along [01] \( \rho a'm \)  
\( a^* = b \)  
\( a^* = a/2 \)  
Origin at x,0  
Origin at 0,y
Origin on 2'1g'

Asymmetric unit  \( 0 \leq x \leq 1/4; \ 0 \leq y \leq 1 \)

Symmetry operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad g' (1/2,0) \\
(3) & \quad m' (1/2,0)' \\
(4) & \quad m (1/4,y) \\
(1/0,0) & \quad (2,0,0)' \\
(m_x 1/2,0)' & \quad (m_x 1/2,0)'
\end{align*}
\]
**Generators selected**
(1); t(1,0); t(0,1); (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(2) x̅,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y [u,ν]</td>
</tr>
<tr>
<td></td>
<td>(4) x̅+1/2,y [u,ν]</td>
</tr>
<tr>
<td>2 c .m.</td>
<td>1/4,y [u,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,y [u,0]</td>
</tr>
<tr>
<td>2 b 2′..</td>
<td>0,1/2 [u,v]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2 [u,ν]</td>
</tr>
<tr>
<td>2 a 2′..</td>
<td>0,0 [u,v]</td>
</tr>
<tr>
<td></td>
<td>1/2,0 [u,ν]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] pm1'  
Along [01] pm  
\(a^* = b\)  
\(a^* = a/2\)  
Origin at x,0  
Origin at 0,y
Origin on 21g'

Asymmetric unit  \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1\)

Symmetry operations

For (0,0) + set

1. \((1,0,0)\)  
   \((1/2,0,0)\)

2. \((0,0)\)  
   \((1/2,0)\)  
   \((0,1/2)\)  
   \((1/2,1/2)\)

For (0,1) + set

1. \((0,1)\)  
   \((0,1/2)\)  
   \((1,0)\)  
   \((1/2,1)\)

\(g\) is a rotation by \(90^\circ\) about the origin.

\(m\) is a mirror plane.

\(t\) is a translation by \(1/2\) in the \(x\) direction.

\(x, y, z\) are Cartesian coordinates.
Continued

No. 7.6.36

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generators selected</td>
<td>(1); t(1,0); t(0,1)'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>(0,0)*</th>
<th>(0,1)' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) x̄,y [ū,v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y [u,v]</td>
<td>(4) x̄+1/2,y [ū,v]</td>
</tr>
<tr>
<td>2 c .m'</td>
<td>1/4,y [0,v]</td>
<td>3/4,y [0,v]</td>
</tr>
<tr>
<td>2 b 2'..</td>
<td>0,1/2 [u,v]</td>
<td>1/2,1/2 [ū,v]</td>
</tr>
<tr>
<td>2 a 2..</td>
<td>0,0 [0,0]</td>
<td>1/2,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] \( p_{2a}m \)
- Along [01] \( pm1' \)
- \( a^* = b \)
- \( a^* = a/2 \)
- Origin at x,1/2
- Origin at 0,y
Origin on 21g

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1

Symmetry operations

For (0,0) + set
(1) 1 (0,0) (2) 2 0,0 (3) g (1/2,0) x,0 (4) m 1/4,y
(1') 0,0 (2') 0,0 (3') 1/2,0 x,1/2 (4') 0,1 1/4,y

For (0,1)' + set
(1) t' (0,1) (2) t 0,1/2 (3) g' (1/2,0) x,1/2 (4) g' (0,1) 1/4,y
(1') 0,1 (2') 0,1/2 (3') 1/2,0 x,1/2 (4') 1/2,1 1/4,y

TABLE 3 - 2D -73
**Generators selected** (1); t(1,0); t(0,1)'; (2); (3)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site symmetry</td>
<td></td>
</tr>
<tr>
<td>(0,0)*</td>
<td>(0,1)*</td>
</tr>
<tr>
<td>4 d 1</td>
<td>(1) x,y [u,v] (2) (\bar{x},y [u,v])</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,(\bar{y}) [(\bar{u},v)] (4) (\bar{x}+1/2,y [u,\bar{v}])</td>
</tr>
<tr>
<td>2 c .m.</td>
<td>1/4,(y [u,0]) 3/4,(\bar{y} [u,0])</td>
</tr>
<tr>
<td>2 b 2'..</td>
<td>0,1/2 [u,v] 1/2,1/2 [u,(\bar{v})]</td>
</tr>
<tr>
<td>2 a 2..</td>
<td>0,0 [0,0] 1/2,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th>Along [10] pm1'</th>
<th>Along [01] pm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = b)</td>
<td>(a^* = a/2)</td>
</tr>
<tr>
<td>Origin at x,0</td>
<td>Origin at 0,y</td>
</tr>
</tbody>
</table>

---

**TABLE 3 - 2D -74**
Origin on 211

Asymmetric unit  $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2$

Symmetry operations

(1) $1$
(1:0,0)

(2) $2 \ 0,0$
(2:0,0)

(3) $g \ (1/2,0) \ x,1/4$
(m:1/2,1/2)

(4) $g \ (0,1/2) \ 1/4,y$
(m:1/2,1/2)
**Generators selected**  (1); t(1,0); t(0,1); (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y [u,v]  (2) x̅,y [u̅,v̅]  (3) x+1/2, y+1/2 [u̅,v]  (4) x̅+1/2, y+1/2 [u,v̅]</td>
</tr>
<tr>
<td>2 b 2..</td>
<td>0,1/2 [0,0]  1/2,0 [0,0]</td>
</tr>
<tr>
<td>2 a 2..</td>
<td>0,0 [0,0]  1/2,1/2 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] $p_{2a.m}$  Along [01] $p_{2a.m}$

$a^* = b/2$  $a^* = a/2$

Origin at x,1/4  Origin at 1/4,y
Origin on 2111’

Asymmetric unit  $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2$

Symmetry operations

For 1 + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>g</td>
<td>g'</td>
</tr>
<tr>
<td>(1)</td>
<td>(2)</td>
<td>(3)</td>
<td>(4)</td>
</tr>
<tr>
<td>(1:0,0)</td>
<td>(2:0,0)</td>
<td>(1/2,0)</td>
<td>(0,1/2)</td>
</tr>
<tr>
<td>(m:1/2,1/2)</td>
<td>(m:1/2,1/2)</td>
<td>(m:1/2,1/2)</td>
<td>(m:1/2,1/2)</td>
</tr>
</tbody>
</table>

For 1' + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1'</td>
<td>2'</td>
<td>g'</td>
<td>g'</td>
</tr>
<tr>
<td>(1)</td>
<td>(2)</td>
<td>(3)</td>
<td>(4)</td>
</tr>
<tr>
<td>(1:0,0)'</td>
<td>(2:0,0)'</td>
<td>(1/2,0)</td>
<td>(0,1/2)</td>
</tr>
<tr>
<td>(m:1/2,1/2)'</td>
<td>(m:1/2,1/2)'</td>
<td>(m:1/2,1/2)'</td>
<td>(m:1/2,1/2)'</td>
</tr>
</tbody>
</table>

TABLE 3 - 2D -77
Continued

Generators selected  (1);  t(1,0);  t(0,1);  (2);  (3);  1’

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>1’ +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 11’</td>
<td>(1) x,y [0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y [0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y+1/2 [0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2 [0,0]</td>
</tr>
</tbody>
</table>

| 2 b 2..1’      | 0,1/2 [0,0] |
|                | 1/2,0 [0,0] |

| 2 a 2..1’      | 0,0 [0,0] |
|                | 1/2,1/2 [0,0] |

Symmetry of special projections

- Along [10] pm1’  
  \( a^* = b/2 \)  
  Origin at x,0

- Along [01] pm1’  
  \( a^* = a/2 \)  
  Origin at 0,y

TABLE 3 - 2D -78
**TABLE 3 - 2D - 79**

**p2g'g'**

No. 8.3.40

**2m'm'**

p2g'g'

---

**Origin** on 211

**Asymmetric unit**  $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2$

**Symmetry operations**

1. 1
2. $0,0$
3. $g' (1/2,0) x,1/4$
4. $g' (0,1/2) 1/4,y$

---

TABLE 3 - 2D - 79
**Generators selected**  (1);  t(1,0);  t(0,1);  (2);  (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>c</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x̅,y̅ [u̅,v̅]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+1/2,y+1/2 [u,v]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x̅+1/2,y+1/2 [u̅,v]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,0 [0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0 [0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,1/2 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] pm'  
  \( \mathbf{a^*} = \mathbf{b}/2 \)
  Origin at x,0

- Along [01] pm'  
  \( \mathbf{a^*} = \mathbf{a}/2 \)
  Origin at 0,y

---

**TABLE 3 - 2D -80**
Origin on 2'11

Asymmetric unit  \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2\)

Symmetry operations

(1) 1  
\((1|0,0)\)

(2) 2' 0,0  
\((2_\|_0,0)'\)

(3) g' (1/2,0) x,1/4  
\((m_\|_1/2,1/2)'\)

(4) g (0,1/2) 1/4,y  
\((m_\|_1/2,1/2)\)
Generators selected
(1); t(1,0); t(0,1); (2); (3)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y+1/2 [u,v]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2 [u,v]</td>
</tr>
<tr>
<td>2 b 2'.</td>
<td>0,1/2 [u,v]</td>
</tr>
<tr>
<td></td>
<td>1/2,0 [u,v]</td>
</tr>
<tr>
<td>2 a 2'.</td>
<td>0,0 [u,v]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2 [u,v]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] \( p_{2a,m} \)  
Along [01] \( pm \)

\( a^* = b/2 \)  
\( a^* = a/2 \)

Origin at x,0  
Origin at 0,y

TABLE 3 - 2D -82
**Origin** on 2mm

**Asymmetric unit** \(0 \leq x \leq \frac{1}{4}; \ 0 \leq y \leq \frac{1}{2}\)

**Symmetry operations**

For \((0,0)\) + set

\[
\begin{align*}
1 & \quad (0,0) \\
(1) & \quad 2 \quad (0,0) \\
(2) & \quad m \quad x,0 \\
(3) & \quad m \quad 0,y \\
(4) & \quad m \quad 0,0 \\
\end{align*}
\]

For \((1/2,1/2)\) + set

\[
\begin{align*}
1 & \quad (1/2,0) \\
(1) & \quad 2 \quad 1/4,1/4 \\
(2) & \quad 1/4,1/4 \\
(3) & \quad g \quad (1/2,0) \quad x,1/4 \\
(4) & \quad g \quad 0,1/2 \quad 1/4,y \\
\end{align*}
\]

[Diagram of the symmetry operations]
**Generators selected**  
(1); t(1,0); t(0,1); t(1/2,1/2); (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) +</td>
<td>(1/2,1/2) +</td>
</tr>
<tr>
<td>8 f 1</td>
<td></td>
</tr>
<tr>
<td>(1) x,y [u,v]</td>
<td>(2) x̅,y [u̅,v̅]</td>
</tr>
<tr>
<td>(3) x,y [u,v]</td>
<td>(4) x̅,y [u̅,v̅]</td>
</tr>
<tr>
<td>4 e .m.</td>
<td></td>
</tr>
<tr>
<td>0,y [u,0]</td>
<td>0, y̅ [u̅,0]</td>
</tr>
<tr>
<td>4 d ..m</td>
<td></td>
</tr>
<tr>
<td>x,0 [0,v]</td>
<td>x̅,0 [0,v]</td>
</tr>
<tr>
<td>4 c 2..</td>
<td></td>
</tr>
<tr>
<td>1/4,1/4 [0,0]</td>
<td>1/4,3/4 [0,0]</td>
</tr>
<tr>
<td>2 b 2mm</td>
<td></td>
</tr>
<tr>
<td>0,1/2 [0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2mm</td>
<td></td>
</tr>
<tr>
<td>0,0 [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] pm 1'  
Along [01] pm 1'  
\(a^* = b/2\)  
\(a^* = a/2\)  
Origin at x,0  
Origin at 0, y

---

**TABLE 3 - 2D -84**
Origin on 2mm1'

Asymmetric unit  $0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2$

Symmetry operations

For (0,0) + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(1,0,0)</td>
</tr>
<tr>
<td>2</td>
<td>0,0</td>
</tr>
<tr>
<td>m</td>
<td>x,0</td>
</tr>
<tr>
<td>m</td>
<td>0,y</td>
</tr>
</tbody>
</table>

For (1/2,1/2) + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>t</td>
<td>(1/2,1/2)</td>
</tr>
<tr>
<td>2</td>
<td>1/4,1/4</td>
</tr>
<tr>
<td>g</td>
<td>(1/2,0) x,1/4</td>
</tr>
<tr>
<td>g</td>
<td>(0,1/2) 1/4,y</td>
</tr>
</tbody>
</table>

For (0,0)' + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1'</td>
<td>(1,0,0)'</td>
</tr>
<tr>
<td>2'</td>
<td>0,0</td>
</tr>
<tr>
<td>m'</td>
<td>x,0</td>
</tr>
<tr>
<td>m'</td>
<td>0,y</td>
</tr>
</tbody>
</table>

For (1/2,1/2)' + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>t'</td>
<td>(1/2,1/2)</td>
</tr>
<tr>
<td>2'</td>
<td>1/4,1/4</td>
</tr>
<tr>
<td>g'</td>
<td>(1/2,0) x,1/4</td>
</tr>
<tr>
<td>g'</td>
<td>(0,1/2) 1/4,y</td>
</tr>
</tbody>
</table>

TABLE 3 - 2D -85
**Generators selected**  (1);  t(1,0);  t(0,1);  t(1/2,1/2);  (2);  (3);  1'

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) +</td>
<td>(1/2,1/2) +</td>
</tr>
<tr>
<td>(0,0)'+</td>
<td>(1/2,1/2)'+</td>
</tr>
</tbody>
</table>

| 8 | f | 11' | (1) x,y [0,0] | (2) x̅,y [0,0] |
|   |   |     | (3) x,ŷ [0,0] | (4) ŷ,x [0,0] |

| 4 | e | .m.1' | 0,y [0,0] | ŷ,0 [0,0] |

| 4 | d | ..m1' | x,0 [0,0] | ŷ,0 [0,0] |

| 4 | c | 2..1' | 1/4,1/4 [0,0] | 1/4,3/4 [0,0] |

| 2 | b | 2mm1' | 0,1/2 [0,0] |

| 2 | a | 2mm1' | 0,0 [0,0] |

**Symmetry of special projections**

Along [10] pm1'  
\(a^* = b/2\)

Along [01] pm1'  
\(a^* = a/2\)

Origin at x,0  
Origin at 0,y
Origin on 2m’m’

Asymmetric unit  $0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2$

Symmetry operations

For (0,0) + set

(1) $1$  
(2) $2 \ 0,0$  
(3) $m' \ x,0$  
(4) $m' \ 0,y$

For $(1/2,1/2)$ + set

(1) $t \ (1/2,1/2)$  
(2) $2 \ 1/4,1/4$  
(3) $g' \ (1/2,0) \ x,1/4$  
(4) $g' \ (0,1/2) \ 1/4,y$

TABLE 3 - 2D -87
**Generators selected** (1); t(1,0); t(0,1); t(1/2,1/2); (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) +</td>
<td>(1/2,1/2) +</td>
</tr>
</tbody>
</table>

8  f  1  
(1) x,y [u,v]  
(2) \( \bar{x}, \bar{y} [\bar{u}, \bar{v}] \)  
(3) x,\( \bar{y} [u, \bar{v}] \)  
(4) \( \bar{x}, y [\bar{u}, v] \)

4  e  .m'.  0,y [0,v]  0,\( \bar{y} [0, \bar{v}] \)

4  d  .m'  x,0 [u,0]  \( \bar{x}, 0 [\bar{u}, 0] \)

4  c  2..  1/4,1/4 [0,0]  1/4,3/4 [0,0]

2  b  2m'm'  0,1/2 [0,0]

2  a  2m'm'  0,0 [0,0]

**Symmetry of special projections**

Along [10] pm'  Along [01] pm'
\( a^{*} = b/2 \)  \( a^{*} = a/2 \)
Origin at x,0  Origin at 0,y

---

**TABLE 3 - 2D -88**
Origin on 2'mm'

Asymmetric unit \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2\)

Symmetry operations

For \((0,0) + \) set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>(0,0)</td>
</tr>
<tr>
<td>2</td>
<td>2'</td>
<td>(0,0)'</td>
</tr>
<tr>
<td>3</td>
<td>m'</td>
<td>(0,0)'</td>
</tr>
<tr>
<td>4</td>
<td>m</td>
<td>(0,0)</td>
</tr>
</tbody>
</table>

For \((1/2,1/2) + \) set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>t</td>
<td>(1/2,1/2)</td>
</tr>
<tr>
<td>2</td>
<td>2'</td>
<td>(1/4,1/4)</td>
</tr>
<tr>
<td>3</td>
<td>g'</td>
<td>(0,1/2)</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
<td>(0,1/2)</td>
</tr>
</tbody>
</table>

TABLE 3 - 2D -89
### Generators selected

(1); t(1,0); t(0,1); t(1/2,1/2); (2); (3)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) x̄,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(3) x̄,y [u,v]</td>
<td>(4) x,y [u,v̄]</td>
</tr>
<tr>
<td>4 e .m.</td>
<td>0,y [u,0]</td>
<td>0,ȳ [u,0]</td>
</tr>
<tr>
<td>4 d ..m'</td>
<td>x,0 [u,0]</td>
<td>x̄,0 [u,0]</td>
</tr>
<tr>
<td>4 c 2'. .</td>
<td>1/4,1/4 [u,v]</td>
<td>1/4,3/4 [u,v̄]</td>
</tr>
<tr>
<td>2 b 2'mm'</td>
<td>0,1/2 [u,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2'mm'</td>
<td>0,0 [u,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- Along [10] pm1'
  - \( a^* = b/2 \)
  - Origin at x,0

- Along [01] pm
  - \( a^* = a/2 \)
  - Origin at 0,y
Origin on 2mm

Asymmetric unit \( 0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2 \)

Symmetry operations

For \((0,0)\) + set

(1) \( 1 \ \ \ (1|0,0) \)
(2) \( 2 \ 0,0 \ \ (2|0,0) \)
(3) \( m \ x,0 \ \ (m|0,0) \)
(4) \( m \ 0,y \ \ (m|0,0) \)

For \((1/2,1/2)'\) + set

(1) \( t' \ \ (1/2,1/2) \)
(2) \( 2' \ 1/4,1/4 \)
(3) \( g' \ (1/2,0) \ x,1/4 \)
(4) \( g' \ (0,1/2) \ 1/4,y \)

\( \text{TABLE 3 - 2D -91} \)
Generators selected

(1); t(1,0); t(0,1); t(1/2,1/2)'; (2); (3)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) +</td>
<td>(1/2,1/2)'+</td>
</tr>
</tbody>
</table>

| 8 f 1 | 1 | (1) x,y [u,v] | (2) x,y [u,v] |
|       |   | (3) x,y [u,v] | (4) x,y [u,v] |

| 4 e .m. | 0,y [u,0] | 0,y [u,0] |
| 4 d ..m | x,0 [0,v] | x,0 [0,v] |
| 4 c 2'.. | 1/4,1/4 [u,v] | 1/4,3/4 [u,v] |
| 2 b 2mm | 0,1/2 [0,0] |
| 2 a 2mm | 0,0 [0,0] |

Symmetry of special projections

Along [10] pm1'  Along [01] pm1'

a* = b/2  a* = a/2

Origin at x,0  Origin at 0,y
**Origin** on 2mm'

**Asymmetric unit**  \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2\)

**Symmetry operations**

For \((0,0)\) + set

1. \(1\) \hspace{1cm} \(2\) \hspace{1cm} \(3\) \hspace{1cm} \(4\)
   \(0,0\) \hspace{1cm} \(0,0\) \hspace{1cm} \((1/0,0)\) \hspace{1cm} \((m,0,0)\) \hspace{1cm} \((m,0,0)\) \hspace{1cm} \(0,y\)

For \((1/2,1/2)\) + set

1. \(t\) \hspace{1cm} \(2\) \hspace{1cm} \(3\) \hspace{1cm} \(4\)
   \((1/2,1/2)\) \hspace{1cm} \((1/2,1/4)\) \hspace{1cm} \((1/2,0)\) \hspace{1cm} \((0,1/2)\)

   \((1/2,1/2)\) \hspace{1cm} \((1/2,1/4)\) \hspace{1cm} \((m,1/2,1/4)\) \hspace{1cm} \((m,1/2,1/2)\)

   \((1/2,1/2)\) \hspace{1cm} \((1/2,1/4)\) \hspace{1cm} \((m,1/2,1/4)\) \hspace{1cm} \((m,1/2,1/2)\)
Continued

TABLE 3 - 2D - 94

Generators selected
(1); t(1,0); t(0,1); t(1/2,1/2)'; (2); (3)

Positions

<table>
<thead>
<tr>
<th>Symmetry of special projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [10] \rho_{2a}\cdot m</td>
</tr>
<tr>
<td>\mathbf{a}^* = \frac{\mathbf{b}}{2}</td>
</tr>
<tr>
<td>Origin at \mathbf{x},1/4</td>
</tr>
</tbody>
</table>
Origin on 2\textsuperscript{mm}'

Asymmetric unit \(0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2\)

Symmetry operations

For \((0,0) +\) set

(1) \(1\) \(\begin{array}{c}
(0,0) \\
(1,0,0)
\end{array}\)

(2) \(2'\) \(\begin{array}{c}
0,0 \\
(2_2,0,0)'
\end{array}\)

(3) \(m'\) \(\begin{array}{c}
x,0 \\
(m_y,0,0)'
\end{array}\)

(4) \(m\) \(\begin{array}{c}
0,y \\
(m_x,0,0)
\end{array}\)

For \((1/2,1/2)' +\) set

(1) \(t'\) \(\begin{array}{c}
(1/2,1/2) \\
(1,2,1/2)'
\end{array}\)

(2) \(2\) \(\begin{array}{c}
1/4,1/4 \\
(2_2,1/2,1/2)
\end{array}\)

(3) \(g\) \(\begin{array}{c}
(1/2,0) \\
(1,2,1/2)
\end{array}\)

(4) \(g'\) \(\begin{array}{c}
(0,1/2) \\
(m_x,1/2,1/2)
\end{array}\)
**Generators selected**  (1);  t(1,0);  t(0,1);  t(1/2,1/2)'; (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) x̅,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(3) x̅,y [u,v̅]</td>
<td>(4) x̅,y [u,v̅]</td>
</tr>
<tr>
<td>4 e .m.</td>
<td>0,y [u,0]</td>
<td>0,y̅ [u,0]</td>
</tr>
<tr>
<td>4 d ..m'</td>
<td>x,0 [u,0]</td>
<td>x̅,0 [u,0]</td>
</tr>
<tr>
<td>4 c 2..</td>
<td>1/4,1/4 [0,0]</td>
<td>1/4,3/4 [0,0]</td>
</tr>
<tr>
<td>2 b 2'mm'</td>
<td>0,1/2 [u,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2'mm'</td>
<td>0,0 [u,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] p m1'  
-origin at x,0

Along [01] p 2m  
-origin at 0,y
Origin on 4

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2

Symmetry operations

(1) 1  (2) 2  0,0  (3) 4*  0,0  (4) 4*  0,0
(1|0,0) (2|0,0) (4z|0,0) (4z |0,0)
Continued

**Table 3 - 2D - 98**

**Generators selected**
(1); t(1,0); t(0,1); (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y [u,v] (2) x, y [u,v] (3) y,x [v,u] (4) y,x [v,u]</td>
</tr>
<tr>
<td>2 c 2..</td>
<td>0,1/2 [0,0] 1/2,0 [0,0]</td>
</tr>
<tr>
<td>1 b 4..</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>1 a 4..</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**


\[ a^* = b \quad a^* = (-a+b)/2 \]

Origin at x,0  Origin at x,x
Origin on 41'

Asymmetric unit  \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2 \)

Symmetry operations

For 1 + set

(1) 1  
\( (1,0,0) \)

(2) 2  0,0  
\( (2z,0,0) \)

(3) 4^+  0,0  
\( (4z,0,0) \)

(4) 4^-  0,0  
\( (4z^{-1},0,0) \)

For 1' + set

(1) 1'  
\( (1,0,0)' \)

(2) 2'  0,0  
\( (2z,0,0)' \)

(3) 4'^+  0,0  
\( (4z,0,0)' \)

(4) 4'^-  0,0  
\( (4z^{-1},0,0)' \)
**Generators selected**  (1); t(1,0); t(0,1); (2); (3); 1’

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>d</td>
<td>11’</td>
</tr>
<tr>
<td>1’+</td>
<td>d</td>
<td>11’</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>21’</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>41’</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>41’</td>
</tr>
</tbody>
</table>

**Coordinates**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>d</td>
<td>11’</td>
<td>(1) x, y [0,0]</td>
</tr>
<tr>
<td>1’+</td>
<td>d</td>
<td>11’</td>
<td>(2) x̅, y [0,0]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>21’</td>
<td>(3) y, x [0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>41’</td>
<td>(4) y, x̅ [0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>41’</td>
<td>0, 0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- **Along [10] pm1’**
  - a* = b
  - Origin at x, 0
- **Along [11] pm1’**
  - a* = (-a + b) / 2
  - Origin at x, x
Origin on 4'

Asymmetric unit  $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2$

Symmetry operations

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>1</td>
<td>(2)</td>
<td>2 0.0</td>
</tr>
<tr>
<td>(1)</td>
<td>(0,0)</td>
<td>(2)</td>
<td>(z,0)</td>
</tr>
<tr>
<td>(3)</td>
<td>4+, 0,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4)</td>
<td>4-, 0,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4)</td>
<td>(4,0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4)</td>
<td>(4,1,0)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

TABLE 3 - 2D -101
**Generators selected** (1); t(1,0,0); t(0,1,0); (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4  d  1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td>2  c  2..</td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td>1  b  4'..</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>1  a  4'..</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>a* =(-a+b)/2</td>
</tr>
<tr>
<td>Origin at x,0</td>
<td>Origin at x,x</td>
</tr>
</tbody>
</table>
Origin on 4

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2

Symmetry operations

For (0,0) + set
(1) 1 0,0
(2) 2 0,0
(3) 4+ 0,0
(4) 4− 0,0

For (1,0)' + set
(1) t' (1,0)
(2) 2' 1/2,0
(3) 4+ ' 1/2,1/2
(4) 4− ' 1/2,1/2

TABLE 3 - 2D -103
**Generators selected** (1); t(1,0)'; t(0,1)'; (2); (3)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0)*</td>
<td>(1,0)’*</td>
</tr>
<tr>
<td>4 d 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td>2 C 2’..</td>
<td>0,1/2 [u,v]</td>
</tr>
<tr>
<td>1 B 4’..</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>1 A 4’..</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] $p_{2a}m$: $a^* = b$
- Origin at $x,1/2$
- Origin at $x-1/4,x+1/4$

---

TABLE 3 - 2D -104
### Origin on 4mm

**Asymmetric unit**  \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ x \leq y\)

**Symmetry operations**

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>(1</td>
</tr>
<tr>
<td>2</td>
<td>2 0,0</td>
<td>(2</td>
</tr>
<tr>
<td>3</td>
<td>4+ 0,0</td>
<td>(4</td>
</tr>
<tr>
<td>4</td>
<td>4− 0,0</td>
<td>(4</td>
</tr>
<tr>
<td>5</td>
<td>m x,0</td>
<td>(m</td>
</tr>
<tr>
<td>6</td>
<td>m 0,y</td>
<td>(m</td>
</tr>
<tr>
<td>7</td>
<td>m x,x</td>
<td>(m</td>
</tr>
<tr>
<td>8</td>
<td>m x,x</td>
<td>(m</td>
</tr>
</tbody>
</table>
**Generators selected** (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 8 g 1    | (1) x,y [u,v]  
           | (2) x̅,y [u̅,v]  
           | (3) y,x [v,u]  
           | (4) y,x [v,u̅]  
           | (5) x,y [u,v]  
           | (6) x̅,y [u̅,v]  
           | (7) x̅,x [u,u̅]  
           | (8) x,y [v,u̅] |
| 4 f .m.  | x,1/2 [0,v]  
           | x̅,1/2 [0,v̅]  
           | 1/2,x [v̅,0]  
           | 1/2,x [v,0] |
| 4 e .m.  | x,0 [0,v]  
           | x̅,0 [0,v̅]  
           | 0,x [v̅,0]  
           | 0,x [v,0] |
| 4 d ..m | x,x [u̅,u]  
           | x̅,x [u̅,u]  
           | x,x [u,u]  
           | x,x [u,u] |
| 2 c 2mm. | 1/2,0 [0,0]  
           | 0,1/2 [0,0] |
| 1 b 4mm  | 1/2,1/2 [0,0] |
| 1 a 4mm  | 0,0 [0,0] |

**Symmetry of special projections**

- Along [10] pm1'  
  - $a^* = b$
  - $a^* = (-a+b)/2$
- Along [11] pm1'  
  - Origin at x,0  
  - Origin at x,x
**Origin on 4mm1’**

**Asymmetric unit**  $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ x \leq y$

**Symmetry operations**

<table>
<thead>
<tr>
<th>Set</th>
<th>1</th>
<th>2   0,0</th>
<th>4   0,0</th>
<th>4’  0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>For 1’ + set</td>
<td>1’</td>
<td>2’  0,0</td>
<td>4’ 0,0</td>
<td>4’  0,0</td>
</tr>
<tr>
<td>(1) m’ x,0</td>
<td>m’ 0,y</td>
<td>m’ x,\bar{x}</td>
<td>m’ x,x</td>
<td></td>
</tr>
<tr>
<td>(5) m’ 0,0</td>
<td>m’ 0,0</td>
<td>m’ 0,0</td>
<td>m’ 0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Set</th>
<th>1</th>
<th>2   0,0</th>
<th>4   0,0</th>
<th>4’  0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>For 1 + set</td>
<td>1</td>
<td>2   0,0</td>
<td>4   0,0</td>
<td>4’  0,0</td>
</tr>
<tr>
<td>(1) m  x,0</td>
<td>m  0,y</td>
<td>m  x,\bar{x}</td>
<td>m  x,x</td>
<td></td>
</tr>
<tr>
<td>(5) m 0,0</td>
<td>m 0,0</td>
<td>m 0,0</td>
<td>m 0,0</td>
<td></td>
</tr>
</tbody>
</table>

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**TABLE 3 - 2D - 107**
Continued

Generators selected
(1); t(1,0); t(0,1); (2); (3); (5); 1'

Positions

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
<th>1+</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 11'</td>
<td>(1) x,y [0,0]</td>
<td>(2) (\bar{x},\bar{y} [0,0])</td>
<td>(3) (\bar{y},x [0,0])</td>
</tr>
<tr>
<td></td>
<td>(5) x,(\bar{y} [0,0])</td>
<td>(6) x,y [0,0]</td>
<td>(7) (\bar{y},\bar{x} [0,0])</td>
</tr>
<tr>
<td>4 f .m.1'</td>
<td>x,1/2 [0,0]</td>
<td>(\bar{x},1/2 [0,0])</td>
<td>1/2,x [0,0]</td>
</tr>
<tr>
<td>4 e .m.1'</td>
<td>x,0 [0,0]</td>
<td>(\bar{x},0 [0,0])</td>
<td>0,x [0,0]</td>
</tr>
<tr>
<td>4 d ..m1'</td>
<td>x,x [0,0]</td>
<td>(\bar{x},\bar{x} [0,0])</td>
<td>(\bar{x},x [0,0])</td>
</tr>
<tr>
<td>2 c 2mm.1'</td>
<td>1/2,0 [0,0]</td>
<td>0,1/2 [0,0]</td>
<td></td>
</tr>
<tr>
<td>1 b 4mm1'</td>
<td>1/2,1/2 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a 4mm1'</td>
<td>0,0 [0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] pm1'  
\(a^* = b\)
 Origin at x,0

Along [11] pm1'  
\(a^* = (-a+b)/2\)
 Origin at x,x

TABLE 3 - 2D -108
### Table 3 - 2D - 109

#### p4m’m’

No. 11.3.55

**Origin on 4m’m’**

**Asymmetric unit**  
$0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ x < y$

**Symmetry operations**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>$1$</td>
</tr>
<tr>
<td>(1</td>
<td>0,0)</td>
</tr>
<tr>
<td>(2) 2 0,0</td>
<td>$2$</td>
</tr>
<tr>
<td>(2z</td>
<td>0,0)</td>
</tr>
<tr>
<td>(3) 4 0,0</td>
<td>$4^+$</td>
</tr>
<tr>
<td>(4z</td>
<td>0,0)</td>
</tr>
<tr>
<td>(4) 4⁻ 0,0</td>
<td></td>
</tr>
<tr>
<td>(4z⁻</td>
<td>0,0)</td>
</tr>
<tr>
<td>(5) m’ x,0</td>
<td>$m'$ x,0</td>
</tr>
<tr>
<td>(m_y</td>
<td>0,0)’</td>
</tr>
<tr>
<td>(6) m’ 0,y</td>
<td>$m'$ 0,y</td>
</tr>
<tr>
<td>(m_z</td>
<td>0,0)’</td>
</tr>
<tr>
<td>(7) m’ x,\overline{x}</td>
<td>$m'$ x,\overline{x}</td>
</tr>
<tr>
<td>(m_y</td>
<td>0,0)’</td>
</tr>
<tr>
<td>(8) m’ x,x</td>
<td>$m'$ x,x</td>
</tr>
<tr>
<td>(m_z</td>
<td>0,0)’</td>
</tr>
</tbody>
</table>
Generators selected (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(5) x,$\bar{y}$ [u,$\bar{v}$]</td>
</tr>
<tr>
<td>4 f .m'</td>
<td>x,1/2 [u,0]</td>
</tr>
<tr>
<td>4 e .m'</td>
<td>x,0 [u,0]</td>
</tr>
<tr>
<td>4 d ..m'</td>
<td>x,x [u,u]</td>
</tr>
<tr>
<td>2 c 2mm'</td>
<td>1/2,0 [0,0]</td>
</tr>
<tr>
<td>1 b 4m'm'</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>1 a 4m'm'</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] p$\bar{m}$'

| a* = b                         | a* =(-a+b)/2     |
| Origin at x,0                  | Origin at x,x    |

TABLE 3 - 2D -110
TABLE 3 - 2D - 111

p4'mm'                             4'mm'
No. 11.4.56                                                     p4'mm'

Origin on 4'mm'

Asymmetric unit  0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; x ≤ y

Symmetry operations

(1) 1      (2) 2   0,0       (3) 4  '  0,0       (4) 4  '   0,0
       (1|0,0)   (2|0,0)      (4|0,0)'    (4|0,0)'

(5) m   x,0      (6) m   0,y       (7) m  '  x,\bar{x}     (8) m  '  x,x
       (m_y|0,0)   (m_x|0,0)      (m_{x\bar{y}}|0,0)'    (m_{x\bar{y}}|0,0)'

TABLE 3 - 2D - 111
Continued

No. 11.4.56

p4’mm’

**Generators selected**  (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>4 f .m.</td>
<td>x,1/2 [0,v]</td>
</tr>
<tr>
<td>4 e .m.</td>
<td>x,0 [0,v]</td>
</tr>
<tr>
<td>4 d ..m’</td>
<td>x,x [u,u]</td>
</tr>
<tr>
<td>2 c 2mm.</td>
<td>1/2,0 [0,0]</td>
</tr>
<tr>
<td>1 b 4’mm’</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>1 a 4’mm’</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**


a* = b  a* = (-a+b)/2

Origin at x,0  Origin at x,x
**TABLE 3 - 2D - 113**

**p4'm'm**

No. 11.5.57

**4'm'm**

p4'm'm

**Origin** on 4’m’m

**Asymmetric unit** 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; x ≤ y

**Symmetry operations**

- (1) 1
  - (1|0,0)

- (2) 2 0,0
  - (2z|0,0)

- (3) 4*’ 0,0
  - (4z|0,0)'

- (4) 4*’ 0,0
  - (4z'|0,0)'

- (5) m' x,0
  - (my|0,0)'

- (6) m' 0,y
  - (mx|0,0)'

- (7) m x,x
  - (my,x|0,0)

- (8) m x,x
  - (mx,y|0,0)
**Generators selected**  (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1 (1) x,y [u,v]</td>
<td>(2) ( \bar{x}, \bar{y} [\bar{u}, \bar{v}] )</td>
</tr>
<tr>
<td>(3) ( y, x [v, \bar{u}] )</td>
<td>(4) ( y, \bar{x} [\bar{v}, u] )</td>
</tr>
<tr>
<td>(5) ( x, \bar{y} [u, \bar{v}] )</td>
<td>(6) ( \bar{x}, y [u, v] )</td>
</tr>
<tr>
<td>(7) ( \bar{y}, x [v, u] )</td>
<td>(8) ( y, x [\bar{v}, \bar{u}] )</td>
</tr>
<tr>
<td>4 f .m'. x,1/2 [u,0]</td>
<td>( \bar{x}, 1/2 [\bar{u}, 0] )</td>
</tr>
<tr>
<td>1/2,x [0,\bar{u}]</td>
<td>1/2,( \bar{x} [0,u] )</td>
</tr>
<tr>
<td>4 e .m'. x,0 [u,0]</td>
<td>( \bar{x}, 0 [\bar{u}, 0] )</td>
</tr>
<tr>
<td>0,x [0,\bar{u}]</td>
<td>0,( \bar{x} [0,u] )</td>
</tr>
<tr>
<td>4 d ..m x,x [u,u]</td>
<td>( \bar{x}, x [\bar{u}, \bar{u}] )</td>
</tr>
<tr>
<td>( \bar{x}, x [u, \bar{u}] )</td>
<td>x,( \bar{x} [\bar{u}, u] )</td>
</tr>
<tr>
<td>2 c 2m'm'. 1/2,0 [0,0]</td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td>1 b 4'm'm 1/2,1/2 [0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a 4'm'm 0,0 [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] \( pm \)
  - \( a^* = b \)
  - Origin at \( x,0 \)

- Along [11] \( pm 1' \)
  - \( a^* = (-a + b)/2 \)
  - Origin at \( x,x \)
TABLE 3 - 2D - 115

\[ \text{Origin on } 4m'm' \]

\[ \text{Asymmetric unit } 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad x \leq y \]

\[ \text{Symmetry operations} \]

For \((0,0) + \text{set}\)

1. \((10,0)\)
2. \((22,0)\)
3. \((40,0)\)
4. \((42,0)\)
5. \((m1,0')\)
6. \((m2,0)\)
7. \((m3,x,x)\)
8. \((m4,0)\)

For \((1,0) + \text{set}\)

1. \((11,0)\)
2. \((22,0)\)
3. \((31,0)\)
4. \((42,0)\)
5. \((g1,0)\)
6. \((m1,1)\)
7. \((m2,1)\)
8. \((m3,1)\)
**Generators selected**  
(1); t(1,0)'; t(0,1)'; (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
<th>(0,0)*</th>
<th>(1,0)*'</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y [u,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x, y [u,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) y, x [v,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) y, x [v,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) x, y [u,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(6) x, y [u,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) y, x [v,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(8) y, x [v,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 f .m.</td>
<td>x,1/2 [0,v]</td>
<td>1/2,x [v,0]</td>
<td>1/2,x [v,0]</td>
</tr>
<tr>
<td></td>
<td>x,1/2 [0,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 e .m'.</td>
<td>x,0 [u,0]</td>
<td>0,x [0,u]</td>
<td>0,x [0,u]</td>
</tr>
<tr>
<td></td>
<td>x,0 [u,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 d .m'</td>
<td>x,x [u,u]</td>
<td>x,x [u,u]</td>
<td>x,x [u,u]</td>
</tr>
<tr>
<td></td>
<td>x,x [u,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 2'mm'.</td>
<td>1/2,0 [u,0]</td>
<td>0,1/2 [0,u]</td>
<td></td>
</tr>
<tr>
<td>1 b 4'm'm</td>
<td>1/2,1/2 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a 4m'm'</td>
<td>0,0 [0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] \( p_{2a}m \)   
Along [11] \( p_{2a}m \)   
\( a^* = b \)   
\( a^* = (-a+b)/2 \)   
Origin at x,1/2   
Origin at x-1/4,x+1/4
Origin on 4mm

Asymmetric unit  \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ x \leq y\)

Symmetry operations

For \((0,0) + set\)

\begin{align*}
(1) & \quad 1 \quad (1'0,0) \\
(2) & \quad 2 \quad 0,0 \quad (2_20,0) \\
(3) & \quad 4' \quad 0,0 \quad (4_20,0) \\
(4) & \quad 4' \quad 0,0 \quad (4_21,0) \\
(5) & \quad m \quad x,0 \quad (m_20,0) \\
(6) & \quad m' \quad 0,y \quad (m_20,0) \\
(7) & \quad m' \quad x,x \quad (m_20,0) \\
(8) & \quad m' \quad x,x \quad (m_20,0)
\end{align*}

For \((1,0)' + set\)

\begin{align*}
(1) & \quad t' \quad (1,0) \\
(2) & \quad 2' \quad 1/2,0 \quad (2_21,0) \\
(3) & \quad 4' \quad 1/2,1/2 \quad (4_21,0) \\
(4) & \quad 4' \quad 1/2,1/2 \quad (4_21,0) \\
(5) & \quad g' \quad (1,0) \quad x,0 \quad (m_20,0) \\
(6) & \quad m' \quad 1/2,0 \quad (m_21,0) \\
(7) & \quad g' \quad (1/2,-1/2) \quad x+1/2 \quad (m_21,0) \\
(8) & \quad g' \quad (1/2,1/2) \quad x+1/2 \quad (m_21,0)
\end{align*}
Continued

| No. 11.7.59 | p_p4mm |

**Generators selected**  
(1); t(1,0)'; t(0,1)'; (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0)*</td>
</tr>
<tr>
<td>8 g 1</td>
<td>x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>x,y [u,v]</td>
</tr>
<tr>
<td>4 f .m'</td>
<td>x,1/2 [u,0]</td>
</tr>
<tr>
<td>4 e .m.</td>
<td>x,0 [0,v]</td>
</tr>
<tr>
<td></td>
<td>x,0 [0,v]</td>
</tr>
<tr>
<td></td>
<td>x,0 [0,v]</td>
</tr>
<tr>
<td>4 d ..m</td>
<td>x,x [u,u]</td>
</tr>
<tr>
<td>2 c 2'm'm.</td>
<td>1/2,0 [0,v]</td>
</tr>
<tr>
<td>1 b 4'm'm</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>1 a 4mm</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = b</td>
<td>a' = (-a+b)/2</td>
</tr>
<tr>
<td>Origin at x,0</td>
<td>Origin at x,x</td>
</tr>
</tbody>
</table>

TABLE 3 - 2D-118
Origin on 41g

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ y \leq 1/2 - x$

Symmetry operations

(1) 1  
(1) 0,0  

(2) 2 0,0  
(2) 0,0  

(3) 4* 0,0  
(3) 0,0  

(4) 4^- 0,0  
(4) 0,0  

(5) g (1/2,0) x,1/4  
(m_y|1/2,1/2)  

(6) g (0,1/2) 1/4,y  
(m_x|1/2,1/2)  

(7) m x+1/2,x  
(m_y|1/2,1/2)  

(8) g (1/2,1/2) x,x  
(m_x|1/2,1/2)  

TABLE 3 - 2D -119
Generators selected  (1); t(1,0); t(0,1); (2); (3); (5)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x [v,u]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x [v,u]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2 [u,v]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2 [u,v]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2 [v,u]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2 [v,u]</td>
</tr>
</tbody>
</table>

| 4 c ..m      | x,x+1/2 [u,u]                |
|              | x,x+1/2 [u,u]                |
|              | x+1/2,x [u,u]                |
|              | x+1/2,x [u,u]                |

| 2 b 2.mm     | 1/2,0 [0,0]                  |
|              | 0,1/2 [0,0]                  |

| 2 a 4..      | 0,0 [0,0]                    |
|              | 1/2,1/2 [0,0]                |

Symmetry of special projections

Along [10] pm A
Along [11] pm1'  
\(a^* = \frac{b}{2}\)  
\(a^* = (-a + b)/2\)

Origin at x,1/2  
Origin at x,x
**Origin on 41g1'**

**Asymmetric unit**  \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ y \leq 1/2 - x\)

**Symmetry operations**

<table>
<thead>
<tr>
<th></th>
<th>For 1 + set</th>
<th>For 1' + set</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(1) 1'</td>
<td></td>
</tr>
<tr>
<td>((1</td>
<td>0,0))</td>
<td>((1</td>
</tr>
<tr>
<td></td>
<td>(2) 2 0,0</td>
<td>(2) 2' 0,0</td>
</tr>
<tr>
<td></td>
<td>((2</td>
<td>0,0))</td>
</tr>
<tr>
<td></td>
<td>(3) (4^+) 0,0</td>
<td>(3) (4^+) 0,0</td>
</tr>
<tr>
<td></td>
<td>((4</td>
<td>0,0))</td>
</tr>
<tr>
<td></td>
<td>(4) (4^-) 0,0</td>
<td>(4) (4^-) 0,0</td>
</tr>
<tr>
<td></td>
<td>((4</td>
<td>^{-1}</td>
</tr>
<tr>
<td>(5) (g) ((1/2,0)) x,1/4</td>
<td>(5) (g') ((1/2,0)) x,1/4</td>
<td></td>
</tr>
<tr>
<td>((m_y</td>
<td>1/2,1/2))</td>
<td>((m_y'</td>
</tr>
<tr>
<td>(6) (g) ((0,1/2)) 1/4,y</td>
<td>(6) (g') ((0,1/2)) 1/4,y</td>
<td></td>
</tr>
<tr>
<td>((m_x</td>
<td>1/2,1/2))</td>
<td>((m_x'</td>
</tr>
<tr>
<td>(7) (m) (x+1/2,\bar{x})</td>
<td>(7) (m') (x+1/2,\bar{x})</td>
<td></td>
</tr>
<tr>
<td>((m_{xy}</td>
<td>1/2,1/2))</td>
<td>((m_{xy}'</td>
</tr>
<tr>
<td>(8) (g) ((1/2,1/2)) x,x</td>
<td>(8) (g') ((1/2,1/2)) x,x</td>
<td></td>
</tr>
<tr>
<td>((m_{xy}</td>
<td>1/2,1/2))</td>
<td>((m_{xy}'</td>
</tr>
</tbody>
</table>
Generators selected  (1); t(1,0); t(0,1); (2); (3); (5); 1’

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+ 1+ +</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Coords</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 11’</td>
<td>(1) x,y [0,0] (2) x̅,y [0,0] (3) y,x [0,0] (4) y,x̅ [0,0] (5) x+1/2,y+1/2 [0,0] (6) x+1/2,y+1/2 [0,0] (7) y+1/2,x+1/2 [0,0] (8) y+1/2,x+1/2 [0,0]</td>
</tr>
<tr>
<td>4 c ..m1’</td>
<td>x,x+1/2 [0,0] x̅,x+1/2 [0,0] x+1/2,x [0,0] x+1/2,x̅ [0,0]</td>
</tr>
<tr>
<td>2 b 2.mm1’</td>
<td>1/2,0 [0,0] 0,1/2 [0,0]</td>
</tr>
<tr>
<td>2 a 4..1’</td>
<td>0,0 [0,0] 1/2,1/2 [0,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections


a* = b/2 a* =(-a+b)/2

Origin at x,0 Origin at x,x
**TABLE 3 - 2D - 123**

**Origin** on 41g'

**Asymmetric unit**  
\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad y \leq 1/2 - x \]

**Symmetry operations**

1. \( 1 \)  
   \[ (1) \begin{pmatrix} 1 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

2. \( 2 \)  
   \[ (2) \begin{pmatrix} 2 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

3. \( 4^+ \)  
   \[ (3) \begin{pmatrix} 4 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

4. \( 4^- \)  
   \[ (4) \begin{pmatrix} 4 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

5. \( g' \)  
   \[ (5) \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

6. \( g' \)  
   \[ (6) \begin{pmatrix} 0 \end{pmatrix} \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

7. \( m' \)  
   \[ (7) m' x+1/2,x \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

8. \( g' \)  
   \[ (8) g' \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} x \end{pmatrix} \begin{pmatrix} x \end{pmatrix} \]

\[ (m_{y}) \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]

\[ (m_{xy}) \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 0 \end{pmatrix} \]
Generators selected: (1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y [u,v] (2) x̅,y̅ [u̅,v̅]</td>
</tr>
<tr>
<td></td>
<td>(3) y̅,x [v̅,u] (4) y,x [v,u]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2 [u,v] (6) x̅+1/2,y+1/2 [u̅,v̅]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2 [v̅,u̅] (8) y+1/2,x+1/2 [v,u]</td>
</tr>
<tr>
<td>4 c ..m'</td>
<td>x,x+1/2 [u,u] x̅,x̅+1/2 [u̅,u̅] x̅+1/2,x [u̅,u] x+1/2,x [u,u]</td>
</tr>
<tr>
<td>2 b 2.m'm'</td>
<td>1/2,0 [0,0] 0,1/2 [0,0]</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0 [0,0] 1/2,1/2 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**


a* = b/2 a* =(-a+b)/2

Origin at x,0 Origin at x,x

---

**TABLE 3 - 2D -124**
**TABLE 3 - 2D - 125**

**p4'gm'**

No. 12.4.63

**Asymmetric unit**

$0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ y \leq 1/2 - x$

**Symmetry operations**

1. $1$
   
2. $2 \ 0,0$
   
3. $4^{+} \ 0,0$
   
4. $4^{-} \ 0,0$
5. $g \ (1/2,0) \ x, 1/4$
6. $g \ (0,1/2) \ 1/4, y$
7. $m' \ x+1/2, \bar{x}$
8. $g' \ (1/2,1/2,0) \ x,x$

**Origin on 4'1g'**
**Continued**

**No. 12.4.63**

**p4’gm’**

**Generators selected**

(1); t(1,0); t(0,1); (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(2) x̅,y̅ [u̅,v̅]</td>
</tr>
<tr>
<td></td>
<td>(3) y̅,x [v̅,u̅]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x [v,u]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2 [u̅,v̅]</td>
</tr>
<tr>
<td></td>
<td>(6) x̅+1/2,y̅+1/2 [u̅,v̅]</td>
</tr>
<tr>
<td></td>
<td>(7) y̅+1/2,x̅+1/2 [v̅,u̅]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2 [v,u]</td>
</tr>
<tr>
<td>4 c .m’</td>
<td>x,x+1/2 [u,u]</td>
</tr>
<tr>
<td></td>
<td>x̅,x̅+1/2 [u̅,u̅]</td>
</tr>
<tr>
<td></td>
<td>x̅+1/2,x [u̅,u̅]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x̅ [u,u̅]</td>
</tr>
<tr>
<td>2 b 2.mm</td>
<td>1/2,0 [0,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td>2 a 4’..</td>
<td>0,0 [0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] \(p_{2am}\)  
- Along [11] \(pm\)  
- \(a^* = b/2\)  
- \(a^* = -a+b)/2\)

Origin at x,0  
Origin at x,x
**Origin on 4'1g**

**Asymmetric unit** \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; y \leq 1/2 - x\)

**Symmetry operations**

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(1) ((1;0,0))</td>
</tr>
<tr>
<td>2</td>
<td>(2) ((0,0))</td>
</tr>
<tr>
<td>3</td>
<td>(4') ((0,0))</td>
</tr>
<tr>
<td>4</td>
<td>(4') ((0,0))</td>
</tr>
<tr>
<td>5</td>
<td>(g') ((1/2,0)) (x,1/4) ((m_y,1/2,1/2))</td>
</tr>
<tr>
<td>6</td>
<td>(g') ((0,1/2)) (1/4,y) ((m_x,1/2,1/2))</td>
</tr>
<tr>
<td>7</td>
<td>(m) (x+1/2,\bar{x}) ((m_x,1/2,1/2))</td>
</tr>
<tr>
<td>8</td>
<td>(g) ((1/2,1/2)) (x,x) ((m_y,1/2,1/2))</td>
</tr>
</tbody>
</table>
Generators selected  
(1): t(1,0);  t(0,1);  (2): (3);  (5)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y [u,v]     (2) x,¯y [u,¯v]</td>
</tr>
<tr>
<td></td>
<td>(3) y, x [v,¯u]   (4) y,¯x [v,u]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2, y+1/2 [u,¯v]  (6) x+1/2, y+1/2 [u,v]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2, x+1/2 [v,u]  (8) y+1/2, x+1/2 [v,¯u]</td>
</tr>
<tr>
<td>4 c .m</td>
<td>x,x+1/2 [u,¯u]     x,x+1/2 [u,¯u]     x+1/2,x [u,u]     x+1/2,x [u,¯u]</td>
</tr>
<tr>
<td>2 b 2.mm</td>
<td>1/2,0 [0,0]        0,1/2 [0,0]</td>
</tr>
<tr>
<td>2 a 4'..</td>
<td>0,0 [0,0]          1/2,1/2 [0,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] pm  
Along [11] pm1'  
\( a^* = b/2 \)  
\( a^* = (-a+b)/2 \)  
Origin at x,0  
Origin at x,x  

TABLE 3 - 2D -128
Origin on 3

Asymmetric unit  0 ≤ x ≤ 2/3;  0 ≤ y ≤ 2/3;  x ≤ (1 + y)/2;
                 y ≤ min(1 - x, (1 + x)/2)

Vertices  0,0;  1/2,0;  2/3,1/3;  1/3,2/3;  0,1/2

Symmetry operations

(1) 1  
    (1|0,0)  

(2) 3^+ 0,0  
    (3_z|0,0)  

(3) 3^- 0,0  
    (3_z^{-1}|0,0)
### Generators selected
(1); t(1,0); t(0,1); (2)

### Positions

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 d 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(2) y-x-y [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x [u+v,\bar{u}]</td>
</tr>
<tr>
<td>1 c 3..</td>
<td>2/3,1/3 [0,0]</td>
</tr>
<tr>
<td>1 b 3..</td>
<td>1/3,2/3 [0,0]</td>
</tr>
<tr>
<td>1 a 3..</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- Along [10] p1
- Along [21] p1

\[ a^* = (a+2b)/2 \]
\[ a^* = b/2 \]

- Origin at x,0
- Origin at x,x/2
**Origin** on 31'

**Asymmetric unit** 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; x ≤ (1 + y)/2;

\[ y \leq \min(1 - x, (1 + x)/2) \]

**Vertices** 0,0; 1/2,0; 2/3,1/3; 1/3,2/3; 0,1/2

**Symmetry operations**

For 1 + set

1. \( (1,0,0) \)
2. \( 3', 0,0 \)
3. \( 3', 0,0 \)

For 1' + set

1. \( (1,0,0)' \)
2. \( 3'^-, 0,0 \)
3. \( 3'^-, 0,0 \)
Generators selected
(1): t(1,0); t(0,1); (2): 1'

Positions

<table>
<thead>
<tr>
<th>Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td></td>
</tr>
<tr>
<td>1' +</td>
<td></td>
</tr>
<tr>
<td>3 d 11'</td>
<td>(1) x,y [0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) y-x,y [0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x [0,0]</td>
</tr>
<tr>
<td>1 c 3..1</td>
<td>2/3,1/3 [0,0]</td>
</tr>
<tr>
<td>1 b 3..1'</td>
<td>1/3,2/3 [0,0]</td>
</tr>
<tr>
<td>1 a 3..1'</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] p11'  
\( a^* = (a+2b)/2 \)
Origin at x,0

Along [21] p11'
\( a^* = b/2 \)
Origin at x,x/2
Origin on 3m1

Asymmetric unit 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; x ≤ 2y;

y ≤ min(1 - x, 2x)

Vertices 0,0; 2/3,1/3; 1/3,2/3

Symmetry operations

(1) 1
(1|0,0)

(2) 3⁺ 0,0
(3z|0,0)

(3) 3⁻ 0,0
(3z⁻¹|0,0)

(4) m x,x̄
(mₓ|0,0)

(5) m x,2x
(mₓ|0,0)

(6) m 2x,x
(mᵧ|0,0)
Generators selected: (1); t(1,0); t(0,1); (2); (4)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site symmetry</td>
<td></td>
</tr>
</tbody>
</table>

| 6 e 1 | (1) x, y [u, v] | (2) y, x-y [v, u-v] | (3) x+y, x [u+v, u] |
|       |               | (4) y, x [v, u]    | (5) x+y, y [u-v, v] |
|       |               | (6) x, x-y [u, u]  | (7) x, x [u, u]     |

| 3 d m. | x, x [u, u]   | x, 2x [u, 0]       | 2x, x, [0, 0]      |

| 1 c 3m. | 2/3, 1/3 [0, 0] |
| 1 b 3m. | 1/3, 2/3 [0, 0] |
| 1 a 3m. | 0, 0 [0, 0]    |

Symmetry of special projections

a* = (a+2b)/2 a* = b/2
Origin at x, 0 Origin at x, x/2

TABLE 3 - 2D - 134
**Origin** on 3m11′

**Asymmetric unit**  
\[0 \leq x \leq 2/3; \ 0 \leq y \leq 2/3; \ x \leq 2y; \]  
\[y \leq \min(1 - x, 2x)\]

**Vertices**  
0,0; 2/3,1/3; 1/3,2/3

**Symmetry operations**

For 1 + set

(1) 1  
(1',0,0)

(2) 3' 0,0  
(3,2,0,0)

(3) 3' 0,0  
(3,2,0,0)

(4) m x,x

m_{x,y}|0,0)

(5) m x,2x

m_{x,y}|0,0)

(6) m 2x,x

m_{x,y}|0,0)

For 1' + set

(1) 1'

(1',0,0)

(2) 3'' 0,0

(3,2,0,0)'

(3) 3'' 0,0

(3,2,0,0)'

(4) m' x,x

m_{x,y}'|0,0)

(5) m' x,2x

m_{x,y}'|0,0)'

(6) m' 2x,x

m_{x,y}'|0,0)'}
Generators selected: \((1); \ t(1,0); \ t(0,1); \ (2); \ (4); \ 1'\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1+)</td>
<td></td>
</tr>
<tr>
<td>(1' +)</td>
<td></td>
</tr>
<tr>
<td>6 e 11'</td>
<td>(1) (x,y\ [0,0])</td>
</tr>
<tr>
<td></td>
<td>(4) (y\bar{x},x [0,0])</td>
</tr>
<tr>
<td>3 d .m.1'</td>
<td>(x,x [0,0])</td>
</tr>
<tr>
<td>1 c 3m.1'</td>
<td>(2/3,1/3 [0,0])</td>
</tr>
<tr>
<td>1 b 3m.1'</td>
<td>(1/3,2/3 [0,0])</td>
</tr>
<tr>
<td>1 a 3m.1'</td>
<td>(0,0 [0,0])</td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- Along [10] \(p11'\): \(a^* = (a+2b)/2\)
- Along [21] \(pm1'\): \(a^* = b/2\)
- Origin at \(x,0\)
- Origin at \(x,x/2\)
**Table 3 - 2D - 137**

**p3m’1**

**No. 14.3.69**

**3m’1**

**p3m’1**

---

**Origin** on 3m’1

**Asymmetric unit**

\[ 0 \leq x \leq 2/3; \ 0 \leq y \leq 2/3; \ x \leq 2y; \ y \leq \min(1 - x, 2x) \]

**Vertices**

\(0,0; \ 2/3,1/3; \ 1/3,2/3\)

**Symmetry operations**

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>(1,0,0)</td>
</tr>
<tr>
<td>2</td>
<td>3 (0)</td>
<td>(3z,0,0)</td>
</tr>
<tr>
<td>3</td>
<td>3 (0)</td>
<td>(3z^{-1},0,0)</td>
</tr>
<tr>
<td>4</td>
<td>m’ (x,\bar{x})</td>
<td>(m_{xy}(0,0))'</td>
</tr>
<tr>
<td>5</td>
<td>m’ (x,2x)</td>
<td>(m_x(0,0))'</td>
</tr>
<tr>
<td>6</td>
<td>m’ (2x,x)</td>
<td>(m_y(0,0))'</td>
</tr>
</tbody>
</table>

---
**Generators selected**  (1); t(1,0); t(0,1); (2); (4)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 e 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x [u+v,u]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x [v,u]</td>
</tr>
<tr>
<td></td>
<td>(5) x+y,y [u+v,v]</td>
</tr>
<tr>
<td></td>
<td>(6) x-x-y [u-u]</td>
</tr>
<tr>
<td>3 d .m'</td>
<td>x,x [u,u]</td>
</tr>
<tr>
<td></td>
<td>x,2x [u,2u]</td>
</tr>
<tr>
<td></td>
<td>2x,x [2u,2u]</td>
</tr>
<tr>
<td>1 c 3m'</td>
<td>2/3,1/3 [0,0]</td>
</tr>
<tr>
<td>1 b 3m'</td>
<td>1/3,2/3 [0,0]</td>
</tr>
<tr>
<td>1 a 3m'</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] p1  
  - \(a^* = (a+2b)/2\)  
  - Origin at x,0
- Along [21] pm'  
  - \(a^* = b/2\)  
  - Origin at x,x/2
Table 3 - 2D - 139

<table>
<thead>
<tr>
<th>Origin</th>
<th>Asymmetric unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>31m</td>
<td>0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; x ≤ (y + 1)/2; y ≤ min(1 - x, x)</td>
</tr>
</tbody>
</table>

| Vertices | 0,0; 1/2,0; 2/3,1/3; 1/2,1/2 |

<table>
<thead>
<tr>
<th>Symmetry operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
</tr>
<tr>
<td>(1</td>
</tr>
<tr>
<td>(2) 3⁺ 0,0</td>
</tr>
<tr>
<td>(3⁺</td>
</tr>
<tr>
<td>(3) 3⁻ 0,0</td>
</tr>
<tr>
<td>(3⁻</td>
</tr>
<tr>
<td>(4) m x,x</td>
</tr>
<tr>
<td>(m₃</td>
</tr>
<tr>
<td>(5) m x,0</td>
</tr>
<tr>
<td>(m₂</td>
</tr>
<tr>
<td>(6) m 0,y</td>
</tr>
<tr>
<td>(m₁</td>
</tr>
</tbody>
</table>
Generators selected \((1); \ t(1,0); \ t(0,1); \ (2); \ (4)\):

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site symmetry</td>
<td></td>
</tr>
<tr>
<td>6 d 1</td>
<td>((1) \ x,y \ [u,v])</td>
</tr>
<tr>
<td></td>
<td>((2) \ \bar{y},x-y \ [\bar{v},u-v])</td>
</tr>
<tr>
<td></td>
<td>((3) \ \bar{x}+y,x \ [\bar{u}+v,\bar{u}])</td>
</tr>
<tr>
<td></td>
<td>((4) \ y,x \ [\bar{v},\bar{u}])</td>
</tr>
<tr>
<td></td>
<td>((5) \ x-y,\bar{y} \ [\bar{u}+v,v])</td>
</tr>
<tr>
<td></td>
<td>((6) \ \bar{x},\bar{x} \ [u,u-v])</td>
</tr>
<tr>
<td>3 c ..m</td>
<td>(x,0 \ [u,2u])</td>
</tr>
<tr>
<td></td>
<td>(0,x \ [2u,\bar{u}])</td>
</tr>
<tr>
<td></td>
<td>(\bar{x},\bar{x} \ [u,\bar{u}])</td>
</tr>
<tr>
<td>2 b 3..</td>
<td>(1/3,2/3 \ [0,0])</td>
</tr>
<tr>
<td></td>
<td>(2/3,1/3 \ [0,0])</td>
</tr>
<tr>
<td>1 a 3.m</td>
<td>(0,0 \ [0,0])</td>
</tr>
</tbody>
</table>

Symmetry of special projections:

Along \([10] pm\) \hspace{1cm} Along \([21] p11'\)
\(a^* = (a+2b)/2\) \hspace{1cm} \(a^* = b/2\)
Origin at \(x,0\) \hspace{1cm} Origin at \(x,x/2\)

**TABLE 3 - 2D -140**
Origin on 31m1'

Asymmetric unit  \( 0 \leq x \leq 2/3; \ 0 \leq y \leq 1/2; \ x \leq (y + 1)/2; \ y \leq \min(1 - x, x) \)

Vertices  0,0;  1/2,0;  2/3,1/3;  1/2,1/2

Symmetry operations

For 1 + set

(1) 1  
(1,0,0)  

(2) 3'  0,0  
(3_z,0,0)  

(4) m  x,x  
(m_3,0,0)  

For 1' + set

(1') 1'  
(1',0,0)  

(2') 3''  0,0  
(3_z',0,0)  

(4') m'  x,x  
(m_3',0,0)  

(3) 3'  0,0  
(3_z',0,0)  

(4) m  x,x  
(m_3,0,0)  

(5) m'  x,x  
(m_3',0,0)  

(6) m  0,y  
(m_1,0,0)  

(6') m'  0,y  
(m_1',0,0)
Continued No. 15.2.71 p31m1’

**Generators selected**  (1); t(1,0); t(0,1); (2); (4); 1’

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>1’ +</td>
</tr>
</tbody>
</table>

| 6  d  11’   | (1) x,y [0,0]   | (2) y̅,x-y [0,0] | (3) x̅+y,y [0,0] |
|            | (4) y,x [0,0]   | (5) x-y,y [0,0]  | (6) x, x+y [0,0] |

| 3  c  3.m1’ | x,0 [0,0]      | 0,x [0,0]        | x̅,x [0,0]       |

| 2  b  3..1’ | 1/3, 2/3 [0,0] | 2/3, 1/3 [0,0]   |

| 1  a  3.m1’ | 0,0 [0,0]      |

**Symmetry of special projections**

- Along [10] *pm1’*  
  - a* = (a+2b)/2
  - a* = b/2
  - Origin at x,0

- Along [21] *p11’*  
  - Origin at x,x/2

---

TABLE 3 - 2D -142
Origin on 31m'

Asymmetric unit 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; x ≤ (y + 1)/2;
y ≤ min(1 - x, x)

Vertices 0,0; 1/2,0; 2/3,1/3; 1/2,1/2

Symmetry operations

(1) 1
   (1|0,0)
(2) 3^+ 0,0
    (3_z|0,0)
(3) 3^- 0,0
    (3_z^-1|0,0)
(4) m' x,x
    (m_3|0,0)'
(5) m' x,0
    (m_2|0,0)'
(6) m' 0,y
    (m_1|0,0)'
### Generators selected

(1); t(1,0); t(0,1); (2); (4)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 d 1</td>
<td>[(1) x,y [u,v] ]</td>
</tr>
<tr>
<td></td>
<td>[(2) \bar{y},x-y [\bar{v},u-v] ]</td>
</tr>
<tr>
<td></td>
<td>[(3) \bar{x}+y,\bar{x} [\bar{u}+v,\bar{u}] ]</td>
</tr>
<tr>
<td></td>
<td>[(4) y,x [v,u] ]</td>
</tr>
<tr>
<td></td>
<td>[(5) x-y,\bar{y} [u-v,\bar{v}] ]</td>
</tr>
<tr>
<td></td>
<td>[(6) \bar{x},\bar{x}+y [\bar{u},\bar{u}+v] ]</td>
</tr>
<tr>
<td>3 c ..m'</td>
<td>[x,0 [u,0] ]</td>
</tr>
<tr>
<td></td>
<td>[0,x [0,u] ]</td>
</tr>
<tr>
<td></td>
<td>[\bar{x},\bar{x} [\bar{u},\bar{u}] ]</td>
</tr>
<tr>
<td>2 b 3..</td>
<td>[1/3,2/3 [0,0] ]</td>
</tr>
<tr>
<td></td>
<td>[2/3,1/3 [0,0] ]</td>
</tr>
<tr>
<td>1 a 3.m'</td>
<td>[0,0 [0,0] ]</td>
</tr>
</tbody>
</table>

#### Symmetry of special projections

Along [10] \(p_m'\) 
- \(a^* = (a+2b)/2\)
- Origin at \(x,0\)

Along [21] \(p1\) 
- \(a^* = b/2\)
- Origin at \(x,x/2\)
TABLE 3 - 2D - 145

No. 16. 1.73

Origin on 6

Asymmetric unit 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; x ≤ (1 + y)/2;

y ≤ min(1 - x, x)

Vertices 0,0; 1/2,0; 2/3,1/3; 1/2,1/2

Symmetry operations

(1) 1

(2) 3^+ 0,0

(3) 3^- 0,0

(4) 2 0,0

(5) 6^+ 0,0

(6) 6^- 0,0

(1*|0,0) (3z|0,0) (3^-1|0,0)

(2z|0,0) (6z|0,0) (6z^-1|0,0)

TABLE 3 - 2D - 145
**Generators selected**  (1);  t(1,0);  t(0,1);  (2);  (4)  

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinating</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 d 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) y, x-y [v,u-v]</td>
<td>(3) x+y,x [u+v,u]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y [u,v]</td>
<td>(5) y, x+y [v,u+v]</td>
<td>(6) x-y,x [u-v,u]</td>
</tr>
<tr>
<td>3 c 2..</td>
<td>1/2,0 [0,0]</td>
<td>0,1/2 [0,0]</td>
<td>1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>2 b 3..</td>
<td>1/3,2/3 [0,0]</td>
<td>2/3,1/3 [0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a 6..</td>
<td>0,0 [0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] pm'  
Along [11] pm'  
a* = (a+2b)/2  a* = b/2  
Origin at x,0  Origin at x,x/2
TABLE 3 - 2D - 147

Origin on 61'

Asymmetric unit  \(0 \leq x \leq 2/3; \ 0 \leq y \leq 1/2; \ x \leq (1+y)/2;
\ny \leq \min(1-x, x)\n
Vertices  0,0;  1/2,0;  2/3,1/3;  1/2,1/2

Symmetry operations

For 1 + set

(1) 1
(1,0,0)

(2) 3' 0,0
(3' 0,0)

(3) 3' 0,0
(3' 0,0)

(4) 2 0,0
(2,0,0)

(5) 6' 0,0
(6' 0,0)

(6) 6' 0,0
(6' 0,0)

For 1' + set

(1) 1'
(1,0,0)'

(2) 3'' 0,0
(3'' 0,0)'

(3) 3'' 0,0
(3'' 0,0)'

(4) 2' 0,0
(2',0,0)'

(5) 6'' 0,0
(6'',0,0)'

(6) 6'' 0,0
(6'',0,0)'

TABLE 3 - 2D - 147
**Generators selected**  (1);  t(1,0);  t(0,1);  (2);  (4);  1’

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>1’ +</td>
</tr>
<tr>
<td>6 d 11’</td>
<td>(1) x,y [0,0] (2) y,x-y [0,0] (3) x+y,x [0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y [0,0] (5) y,x+y [0,0] (6) x-y,x [0,0]</td>
</tr>
<tr>
<td>3 c 2..1’</td>
<td>1/2,0 [0,0] 0,1/2 [0,0] 1/2,1/2 [0,0]</td>
</tr>
<tr>
<td>2 b 3..1’</td>
<td>1/3,2/3 [0,0] 2/3,1/3 [0,0]</td>
</tr>
<tr>
<td>1 a 6..1’</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

Along [10] \( p\overline{m} 1' \)  
Along [21] \( p\overline{m} 1' \)  
\( a^* = (a+2b)/2 \)  
\( a^* = b/2 \)  
Origin at x,0  
Origin at x,x/2

---

TABLE 3 - 2D -148
Origin on 6'

Asymmetric unit  \(0 \leq x \leq 2/3; 0 \leq y \leq 1/2; x \leq (1 + y)/2; y \leq \min(1 - x, x)\)

Vertices 0,0; 1/2,0; 2/3,1/3; 1/2,1/2

Symmetry operations

(1) 1  
(1)*0,0  
(1)*0,0

(2) 3 z 0,0  
(3) 3 -1 z 0,0  
(4) 2' 0,0  
(2) 0,0'  
(5) 6 -1 z 0,0  
(6) 6 -1 z 0,0  
(2) 0,0'  
(2) 0,0'

\[\begin{align*}
\text{TABLE 3 - 2D -149}\end{align*}\]
Continued No. 16.3.75 p6’

**Generators selected**  (1); t(1,0); t(0,1); (2); (4)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 d 1</td>
<td>(1) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(2) y-x [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y [u+v,u]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y [u,v]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y [u+v,u]</td>
</tr>
<tr>
<td>3 c 2’..</td>
<td>1/2,0 [u,v]</td>
</tr>
<tr>
<td></td>
<td>0,1/2 [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2 [u+v,u]</td>
</tr>
<tr>
<td>2 b 3..</td>
<td>1/3,2/3 [0,0]</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3 [0,0]</td>
</tr>
<tr>
<td>1 a 6’..</td>
<td>0,0 [0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of special projections**

- Along [10] pm
- Along [21] pm
- \( a^* = \frac{a+2b}{2} \)
- \( a^* = \frac{b}{2} \)
- Origin at x,0
- Origin at x,x/2

**TABLE 3 - 2D -150**
Origin on 6mm

Asymmetric unit  $0 \leq x \leq 2/3; \ 0 \leq y \leq 1/3; \ x \leq (1 + y)/2; \ y \leq x/2$

Vertices  0,0;  1/2,0;  2/3,1/3

Symmetry operations

1. 1
   (1:0,0)
2. 3
   (2:0,0)
3. 3
   (3:0,0)
4. 2
   (4:0,0)
5. 6
   (5:0,0)
6. 6
   (6:0,0)
7. m
   (7:0,0)
8. m
   (8:0,0)
9. m
   (9:0,0)
10. m
    (10:0,0)
11. m
    (11:0,0)
12. m
    (12:0,0)
Generators selected  (1);  t(1,0,0);  t(0,1,0);  (2);  (4);  (7)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12  f 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) y,x-y [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y [u,v]</td>
<td>(5) y,x+y [v,u+v]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x [v,u]</td>
<td>(8) x+y,y [u-v,v]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x [v,u]</td>
<td>(11) x,y,y [u+v,v]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x [u-v,u]</td>
<td>(12) x,x [u,u-v]</td>
</tr>
<tr>
<td>6  e  .m.</td>
<td>x,x [u,u]</td>
<td>x,2x [u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x [u,u]</td>
<td>x,2x [0,u]</td>
</tr>
<tr>
<td>6  d  .m</td>
<td>x,0 [u,2u]</td>
<td>0,x [2u,u]</td>
</tr>
<tr>
<td></td>
<td>0,0 [u,0]</td>
<td>0,0 [2u,u]</td>
</tr>
<tr>
<td>3  c  2mm</td>
<td>1/2,0 [0,0]</td>
<td>0,1/2 [0,0]</td>
</tr>
<tr>
<td>2  b  3m.</td>
<td>1/3,2/3 [0,0]</td>
<td>2/3,1/3 [0,0]</td>
</tr>
<tr>
<td>1  a  6mm</td>
<td>0,0 [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10]  pm1'  Along [21]  pm1'
\( a^* = (a+2b)/2 \)  \( a^* = b/2 \)
Origin at x,0  Origin at x,x/2
Origin on 6mm1'

Asymmetric unit 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/3; x ≤ (1 + y)/2; y ≤ x/2

Vertices 0,0; 1/2,0; 2/3,1/3

Symmetry operations

For 1 + set

1. (1) 1
   (1|0,0)
2. (2) 3* 0,0
   (3z,0,0)
3. (3) 3' 0,0
   (3z',0,0)
4. (4) 2 0,0
   (2z|0,0)
5. (5) 6' 0,0
   (6z',0,0)
6. (6) 6' 0,0
   (6z,0,0)
7. (7) m x,x
   (m_x|0,0)
8. (8) m x,2x
   (m_x,0,0)
9. (9) m 2x,x
   (m_x,0,0)
10. (10) m x,x
    (m_x,0,0)
11. (11) m x,0
    (m_y,0,0)
12. (12) m 0,y
    (m_y,0,0)

TABLE 3 - 2D -153
TABLE 3 - 2D - 154

For 1' + set

<table>
<thead>
<tr>
<th>(1) 1'</th>
<th>(2) 3^+ 0,0</th>
<th>(3) 3^- 0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(11,0,0)'</td>
<td>(3z,0,0)'</td>
<td>(3z^-1,0,0)'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) 2' 0,0</th>
<th>(5) 6^- 0,0</th>
<th>(6) 6^- 0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2z,0,0)'</td>
<td>(6z^-1,0,0)'</td>
<td>(6z,0,0)'</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) m' x,x</th>
<th>(8) m' x,2x</th>
<th>(9) m' 2x,x</th>
</tr>
</thead>
<tbody>
<tr>
<td>(mx,0,0)'</td>
<td>(m,0,0)'</td>
<td>(m,0,0)'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) m' x,x</th>
<th>(11) m' x,0</th>
<th>(12) m' 0,y</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m,0,0)'</td>
<td>(m,0,0)'</td>
<td>(m,0,0)'</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0); t(0,1); (2); (4); (7); 1'

Positions

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+ 1' +</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>12 f 11'</th>
<th>(1) x,y [0,0]</th>
<th>(2) y,x-y [0,0]</th>
<th>(3) x+y,x [0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4) x,y [0,0]</td>
<td>(5) y,x+y [0,0]</td>
<td>(6) x-y,x [0,0]</td>
<td></td>
</tr>
<tr>
<td>(7) y,x [0,0]</td>
<td>(8) x+y,x [0,0]</td>
<td>(9) x,x-y [0,0]</td>
<td></td>
</tr>
<tr>
<td>(10) y,x [0,0]</td>
<td>(11) x-y,y [0,0]</td>
<td>(12) x,x+y [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6 e .m.1'</th>
<th>x,x [0,0]</th>
<th>x,2x [0,0]</th>
<th>2x,x [0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x [0,0]</td>
<td>x,2x [0,0]</td>
<td>2x,x [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6 d .m1'</th>
<th>x,0 [0,0]</th>
<th>0,x [0,0]</th>
<th>x,x [0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,0 [0,0]</td>
<td>0,x [0,0]</td>
<td>x,x [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3 c 2mm1'</th>
<th>1/2,0 [0,0]</th>
<th>0,1/2 [0,0]</th>
<th>1/2,1/2 [0,0]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>2 b 3m.1'</th>
<th>1/3,2/3 [0,0]</th>
<th>2/3,1/3 [0,0]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>1 a 6mm1'</th>
<th>0,0 [0,0]</th>
<th></th>
</tr>
</thead>
</table>
### Symmetry of special projections

<table>
<thead>
<tr>
<th>Along [10] p(m)1'</th>
<th>Along [21] p(m)1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = (a+2b)/2)</td>
<td>(a^* = b/2)</td>
</tr>
<tr>
<td>Origin at x,0</td>
<td>Origin at x,x/2</td>
</tr>
</tbody>
</table>
Table 3 - 2D - 156

**p6m' m'**

No. 17.3.78

**6m' m'**

**Origin** on 6m' m'

**Asymmetric unit** 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/3; x ≤ (1 + y)/2; y ≤ x/2

**Vertices** 0,0; 1/2,0; 2/3,1/3

**Symmetry operations**

1. \(1\) 1
   \(1(0,0)\)

2. \(3^+ 0,0\)
   \(3^+ (0,0)\)

3. \(3^- 0,0\)
   \(3^- (0,0)\)

4. \(2 0,0\)
   \(2(0,0)\)

5. \(6^- 0,0\)
   \(6^- (0,0)\)

6. \(6^- 0,0\)
   \(6^- (0,0)\)

7. \(m' x, x\)
   \(m' (x, 0)\)

8. \(m' x, 2x\)
   \(m' (0, 0)\)

9. \(m' 2x, x\)
   \(m' (0, 0)\)

10. \(m' x, x\)
    \(m' (x, 0)\)

11. \(m' x, x\)
    \(m' (0, 0)\)

12. \(m' x, 0\)
    \(m' (0, 0)\)

---

**TABLE 3 - 2D - 156**
### Generators selected
(1); t(1,0); t(0,1); (2); (4); (7)

### Positions

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
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<td>12 f 1</td>
<td>(1)</td>
<td></td>
</tr>
<tr>
<td>(4) x,y [u,v]</td>
<td>6 e .m'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7) x,y [v,u]</td>
<td>6 d ..m'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(10) y,x [v,u]</td>
<td>3 c 2m'm'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(11) x-y,y [u-v,v]</td>
<td>2 b 3m'</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(12) x-x [u,u]</td>
<td>1 a 6m'm'</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Coordinates

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Origin at x,0</th>
<th>Origin at x,x/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x [u,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,x [0,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x,u [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x,y [u,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>y,x [v,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x-y,y [u-v,v]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>x-x [u,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,0 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/2,0 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,1/2 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1/2,1/2 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2/3,1/3 [0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,0 [0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of special projections

- **Along [10] pm'**
  - \(a' = (a+2b)/2\)
  - \(a' = b/2\)

- **Along [21] pm'**
  - Origin at \(x,0\)
  - Origin at \(x,x/2\)
**Origin** on 6'\text{mm}'

**Asymmetric unit** 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/3; x ≤ (1 + y)/2; y ≤ x/2

**Vertices** 0,0; 1/2,0; 2/3,1/3

**Symmetry operations**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Image</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(1)</td>
<td>0,0</td>
</tr>
<tr>
<td>(2) 3' 0,0</td>
<td>(3)</td>
<td>(3',0,0)</td>
</tr>
<tr>
<td>(4) 2' 0,0</td>
<td>(5)</td>
<td>(2',0,0)'</td>
</tr>
<tr>
<td></td>
<td>(6)</td>
<td>(6',0,0)'</td>
</tr>
<tr>
<td>(7) m x,x</td>
<td>(8)</td>
<td>(m,x,0,0)</td>
</tr>
<tr>
<td></td>
<td>(9)</td>
<td>(m,2x,0,0)</td>
</tr>
<tr>
<td>(10) m' x,x</td>
<td>(11)</td>
<td>(m',x,0,0)'</td>
</tr>
<tr>
<td></td>
<td>(12)</td>
<td>(m',y,0,0)'</td>
</tr>
</tbody>
</table>

*Table 3 - 2D - 158*
**Generators selected**  
(1); t(1,0); t(0,1); (2); (4); (7)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 12 f 1       | (1) x,y [u,v]  
              | (2) y,x-y [v,u-v]  
              | (3) x+y,x [v,u+v]  
              | (4) x,y [u,v]  
              | (5) y,x+y [v,u-v]  
              | (6) x-y,x [u+v,u]  
              | (7) y,x [v,u]  
              | (8) x+y,y [u-v,v]  
              | (9) x,x-y [u,u+v]  
              | (10) y,x [v,u]  
              | (11) x-y,y [v,u]  
              | (12) x,x+y [u,u+v]  

| 6 e .m.      | x,x [u,u]  
              | x,x [u,u]  
              | x,2x [u,0]  
              | x,2x [u,0]  

| 6 d .m'      | x,0 [u,0]  
              | 0,x [u,0]  
              | x,x [u,0]  

| 3 c 2'mm'    | 1/2,0 [u,0]  
              | 0,1/2 [u,0]  

| 2 b 3m.      | 1/3,2/3 [0,0]  

| 1 a 6'mm'    | 0,0 [0,0]  

**Symmetry of special projections**

Along [10] pm1'  
Along [21] pm  
a* = (a+2b)/2  
an* = b/2  
Origin at x,0  
Origin at x,x/2

---

TABLE 3 - 2D -159
Origin on 6\textprime m'\textprime m

Asymmetric unit \(0 \leq x \leq 2/3; \ 0 \leq y \leq 1/3; \ x \leq (1 + y)/2; \ y \leq x/2\)

Vertices \(0,0; \ 1/2,0; \ 2/3,1/3\)

Symmetry operations

\begin{align*}
(1) \ & 1 & 1 \ & 3^+ \ & 0,0 & 3^- \ & 0,0 \\
(1) \ & (1|0,0) & (3_z|0,0) & (3_z^{-1}|0,0) \\
(4) \ & 2' \ & 0,0 & 6^+ \ & 0,0 & 6^{-1} \ & 0,0 \\
(4) \ & (2_z|0,0)' & (6_{z^{-1}}|0,0)' & (6_{z}|0,0)' \\
(7) \ & m' \ & x,\bar{x} & m' \ & 0,2x & m' \ & 2x,x \\
(7) \ & (m_{x'}|0,0)' & (m_{y'}|0,0)' & (m_{y'}|0,0)' \\
(10) \ & m \ & x,x & m \ & 0,0 & y \\
(10) \ & (m_{3}|0,0) & (m_{2}|0,0) & (m_{1}|0,0) \\
\end{align*}
Generators selected

(1); t(1,0); t(0,1); (2); (4); (7)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coords</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 f 1</td>
<td>(1) x,y [u,v]</td>
<td>(2) y,x-y [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y [u,v]</td>
<td>(5) x,y [v,u-v]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y [v,u]</td>
<td>(8) x+y,y [u+v,v]</td>
</tr>
<tr>
<td></td>
<td>(10) x,y [v,u]</td>
<td>(11) x,y,x [u+v,v]</td>
</tr>
<tr>
<td>6 e .m'</td>
<td>x,x [u,u]</td>
<td>x,2x [u,2u]</td>
</tr>
<tr>
<td></td>
<td>x,x [u,u]</td>
<td>x,2x [u,2u]</td>
</tr>
<tr>
<td>6 d .m</td>
<td>x,0 [u,2u]</td>
<td>0,x [2u,u]</td>
</tr>
<tr>
<td></td>
<td>x,0 [u,2u]</td>
<td>0,x [2u,u]</td>
</tr>
<tr>
<td>3 c 2'm'm</td>
<td>1/2,0 [u,2u]</td>
<td>0,1/2 [2u,u]</td>
</tr>
<tr>
<td>2 b 3m'</td>
<td>1/3,2/3 [0,0]</td>
<td>2/3,1/3 [0,0]</td>
</tr>
<tr>
<td>1 a 6'm'm</td>
<td>0,0 [0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of special projections

Along [10] pm

a* = (a+2b)/2

Along [21] pm1'

a* = b/2

Origin at x,0

Origin at x,x/2

TABLE 3 - 2D -161
Table 3 - 3D:

Three-Dimensional Magnetic Space Group Tables

HIERARCHAL THREE DIMENSIONAL MAGNETIC SPACE GROUP SUPERFAMILY INDEX
THREE DIMENSIONAL MAGNETIC SPACE GROUP INDEX

Table 3 - 2D: Two-Dimensional Magnetic Space Group Tables
Table 3 - 1D: One-Dimensional Magnetic Space Group Tables
<table>
<thead>
<tr>
<th>System</th>
<th>Number</th>
<th>Space Group</th>
<th>Number</th>
<th>Space Group</th>
<th>Number</th>
<th>Space Group</th>
<th>Number</th>
<th>Space Group</th>
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</thead>
<tbody>
<tr>
<td><strong>Triclinic System</strong></td>
<td>1</td>
<td>P1</td>
<td>2</td>
<td>P&amp;</td>
<td>3</td>
<td>P2</td>
<td>4</td>
<td>P2_1</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>C2</td>
<td>6</td>
<td>Pm</td>
<td>7</td>
<td>Pc</td>
<td>8</td>
<td>Cm</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>Cc</td>
<td>10</td>
<td>P2/m</td>
<td>11</td>
<td>P2_1/m</td>
<td>12</td>
<td>C2/m</td>
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<tr>
<td></td>
<td>13</td>
<td>P2/c</td>
<td>14</td>
<td>P2_1/c</td>
<td>15</td>
<td>C2/c</td>
<td>16</td>
<td>P222</td>
</tr>
<tr>
<td></td>
<td>17</td>
<td>P222_1</td>
<td>18</td>
<td>P2_2_2</td>
<td>19</td>
<td>P2_2_2_1</td>
<td>20</td>
<td>C222_1</td>
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<td></td>
<td>21</td>
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<td>Pnnn</td>
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<td>Pnna</td>
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<td>Pcca</td>
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<td>Pbam</td>
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<td>61</td>
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<td>66</td>
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<td>Fdd2</td>
<td>69</td>
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**TETRAGONAL SYSTEM**

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**Note:** The above table lists the various crystallographic space groups and their descriptions with corresponding image references. The notation used includes P (primitive), P\& (primitive with inversion), and the superscript numbers indicating the type of symmetry operations.
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| 176.2.1375 | P6$_3$/m1' | 180.4.1399 | P6$_2$'2'2 | 183.9.1423 | P$_{2c}$ 6m'm' |
| 176.3.1376 | P6$_3$/m | 180.5.1400 | P6$_2$'2'2 | | |
| 176.4.1377 | P6$_3$/m' | 180.6.1401 | P$_{2c}$ 6$_2$22 | 184.1.1424 | P6cc |
| 176.5.1378 | P6$_3$'/m' | 180.7.1402 | P$_{2c}$ 6$_2$'2'2 | 184.2.1425 | P6cc1' |
| 177.1.1379 | P622 | 181.1.1403 | P6,22 | 184.3.1426 | P6'c'c |
| 177.2.1380 | P6221' | 181.2.1404 | P$_6$ 221' | 184.4.1427 | P6'cc' |
| 177.3.1381 | P6'2'2 | 181.3.1405 | P$_6$'2'2 | 184.5.1428 | P6'c'c' |
| 177.4.1382 | P6'2'2 | 181.4.1406 | P$_6$'2'2 | | |
| 177.5.1383 | P6'2'2 | 181.5.1407 | P$_6$'2'2 | 185.1.1429 | P6$_3$ cm |
| 177.6.1384 | P$_{2c}$ 622 | 181.6.1408 | P$_{2c}$ 6$_4$22 | 185.2.1430 | P6$_3$ cm1' |
| 177.7.1385 | P$_{2c}$ 6'2'2 | 181.7.1409 | P$_{2c}$ 6$_4$'2'2 | 185.3.1431 | P6$_3$ c'm |
| 178.1.1386 | P6,22 | 182.1.1410 | p6$_3$ 22 | 185.4.1432 | P6$_3$'cm' |
| 178.2.1387 | P6,221' | 182.2.1411 | p6$_3$ 221' | 185.5.1433 | P6$_3$'c'm' |
| 178.3.1388 | P6$_1$'2'2 | 182.3.1412 | p6$_3$'2'2 | 186.1.1434 | P6$_3$ mc |
| 178.4.1389 | P6$_1$'2'2 | 182.4.1413 | p6$_3$'2'2 | 186.2.1435 | P6$_3$ mc1' |
| 178.5.1390 | P6$_1$'2'2 | 182.5.1414 | p6$_3$'2'2 | 186.3.1436 | P6$_3$'m'c |
| 179.1.1391 | P6$_5$ 22 | 183.1.1415 | p6mm | 186.4.1437 | P6$_3$ mc' |
| 179.2.1392 | P6$_5$ 221' | 183.2.1416 | P6mm1' | 186.5.1438 | P6$_3$ m'c' |
| 179.3.1393 | P6$_5$'2'2 | 183.3.1417 | P6'm'm | 187.1.1439 | P6&m2 |
| 179.4.1394 | P6$_5$'2'2 | 183.4.1418 | P6'm'm | 187.2.1440 | P6&m21' |
| 179.5.1395 | P6$_5$ 2'2' | 183.5.1419 | P6'm'm | 187.3.1441 | P6&m'2 |
| 180.1.1396 | P6$_2$ 22 | 183.6.1420 | P$_{2c}$ 6mm | 187.4.1442 | P6&m'2 |
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| 187.6.1444 | P$_{2c}$ 6&m2 | 187.7.1445 | P$_{2c}$ 6&m'2 | | |
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196.1.1506 F23
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197.1.1508 I23
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197.3.1510 I$_p$23
198.1.1511 P2,3
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<td>229.2.1639</td>
</tr>
<tr>
<td>219.6.1593</td>
<td>P̅m̅3̅m</td>
<td>224.7.1617</td>
<td>P̅3̅m̅</td>
<td>229.3.1640</td>
</tr>
<tr>
<td>220.1.1594</td>
<td>P̅m̅3̅m</td>
<td>225.1.1618</td>
<td>Fm̅3̅m</td>
<td>229.4.1641</td>
</tr>
<tr>
<td>220.2.1595</td>
<td>Pm̅3̅m1'</td>
<td>225.2.1619</td>
<td>Fm̅3̅m1'</td>
<td>229.5.1642</td>
</tr>
<tr>
<td>220.3.1596</td>
<td>Pm̅3̅'m</td>
<td>225.3.1620</td>
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<tr>
<td>220.4.1597</td>
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<td>220.5.1598</td>
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<td>225.5.1622</td>
<td>Fm̅3̅'m</td>
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</tr>
<tr>
<td>220.6.1599</td>
<td>P̅m̅ m̅3̅</td>
<td>226.1.1623</td>
<td>Fm̅3̅</td>
<td>229.9.1646</td>
</tr>
<tr>
<td>220.7.1600</td>
<td>P̅m̅ m̅3̅</td>
<td>226.2.1624</td>
<td>Fm̅3̅c</td>
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<tr>
<td>220.8.1601</td>
<td>P̅3̅n</td>
<td>226.2.1625</td>
<td>Fm̅3̅'c</td>
<td>230.2.1648</td>
</tr>
<tr>
<td>220.9.1602</td>
<td>P̅3̅n1'</td>
<td>226.3.1626</td>
<td>Fm̅3̅'c</td>
<td>230.3.1649</td>
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<tr>
<td>220.10.1603</td>
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<td>226.4.1627</td>
<td>Fm̅3̅c'</td>
<td>230.4.1650</td>
</tr>
<tr>
<td>220.11.1604</td>
<td>Pn̅3̅n'</td>
<td>226.5.1628</td>
<td>Fm̅3̅'c'</td>
<td>230.5.1651</td>
</tr>
<tr>
<td>220.12.1605</td>
<td>Pn̅3̅'n'</td>
<td>227.1.1629</td>
<td>Fd̅3̅m</td>
<td>230.1628</td>
</tr>
<tr>
<td>220.13.1606</td>
<td>Pm̅3̅n</td>
<td>227.2.1629</td>
<td>Fd̅3̅m1'</td>
<td></td>
</tr>
</tbody>
</table>
Origin arbitrary

Asymmetric unit \(0 \leq x \leq 1; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1\)

Symmetry Operations

\[(1) \ 1 \quad (1 \ 0,0,0)\]

Generators selected \((1); t(1,0,0); t(0,1,0); t(0,0,1).\)

Positions

Multiplicities, Wyckoff letter, Site Symmetry.

\[
\begin{array}{cccc}
1 & a & 1 & (1) x,y,z \ [u,v,w] \\
\end{array}
\]

Symmetry of Special Projections

Along \([0,0,1] \ p1\) \(a^* = a_p \quad b^* = b_p\)
Origin at 0,0,z

Along \([1,0,0] \ p1\) \(a^* = b_p \quad b^* = c_p\)
Origin at x,0,0

Along \([0,1,0] \ p1\) \(a^* = c_p \quad b^* = a_p\)
Origin at 0,y,0
Triclinic

1.2.2

P11'

11'

Origin
arbitrary

Asymmetric unit
0 < x < 1; 0 < y < 1; 0 < z < 1

Symmetry Operations

For 1 + set

(1) 1
   (1 | 0,0,0)

For 1' + set

(1) 1'
   (1 | 0,0,0')

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

1+ 1'+

1 a 11' (1) x,y,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p11' Along [1,0,0] p11' Along [0,1,0] p11'

\[ a^* = a_p \quad b^* = b_p \]

Origin at 0,0,z

\[ a^* = b_p \quad b^* = c_p \]

Origin at x,0,0

\[ a^* = c_p \quad b^* = a_p \]

Origin at 0,y,0
Origin: arbitrary

Asymmetric unit: $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

(1) $1$

(1) $0,0,0$

For $(0,0,1)' +$ set

(1) $t' \ (0,0,1)$

(1) $0,0,1'$

Generators selected: $(1); t(1,0,0); t(0,1,0); t(0,0,1)'$.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

$(0,0,0) + \quad (0,0,1)' +$

2 a 1 \ (1) $x,y,z [u,v,w]$

Symmetry of Special Projections

Along $[0,0,1]$ \ p11' \ \begin{align*}
\mathbf{a}^* &= \mathbf{a}_p \quad \mathbf{b}^* = \mathbf{b}_p \\
\text{Origin at } 0,0,z
\end{align*}$

Along $[1,0,0]$ \ p_{2a}^{-1} \ \begin{align*}
\mathbf{a}^* &= -\mathbf{c}_p \quad \mathbf{b}^* = \mathbf{b}_p \\
\text{Origin at } x,0,0
\end{align*}$

Along $[0,1,0]$ \ p_{2a}^{-1} \ \begin{align*}
\mathbf{a}^* &= \mathbf{c}_p \quad \mathbf{b}^* = \mathbf{a}_p \\
\text{Origin at } 0,y,0
\end{align*}$
2.1.4 - 1 - 4

**Triclinic**

**Origin**

```
Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1
```

**Symmetry Operations**

1. \( \mathbf{1} \)
2. \( \overline{1} 0,0,0 \)
3. \( (1 0,0,0) \)
4. \( (1 0,0,0) \)

---

**Image Description**

- A diagram illustrating a triclinic crystal lattice with symmetry operations and typical unit cells.
- The origin is marked at \( \overline{1} \).
- Asymmetric unit boundaries are shown with inequalities:
  - 0 ≤ x ≤ 1/2
  - 0 ≤ y ≤ 1
  - 0 ≤ z ≤ 1

---

2.1.4 - 1 - 4
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>1 h 1</td>
<td>1/2,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>1 g 1</td>
<td>0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>1 f 1</td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>1 e 1</td>
<td>1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>1 d 1</td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
<tr>
<td>1 c 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>1 b 1</td>
<td>0,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>1 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1]  p2'11  
  \[a^* = a_p \quad b^* = b_p\]
  Origin at 0,0,z

- Along [1,0,0]  p2'11  
  \[a^* = b_p \quad b^* = c_p\]
  Origin at x,0,0

- Along [0,1,0]  p2'11  
  \[a^* = c_p \quad b^* = a_p\]
  Origin at 0,y,0
Triclinic

2.2.5

$P\bar{1}1'$

$\bar{1}1'$

$P\bar{1}1'$

Origin at $\bar{1}1'$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

Symmetry Operations

For $1 +$ set

(1) $1$

(1) $0,0,0$

(2) $\bar{1}$ $0,0,0$

(1) $0,0,0$

For $1' +$ set

(1) $1'$

(1) $0,0,0'$

(2) $\bar{1}'$ $0,0,0$

(1) $0,0,0'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

Positions

Multiplicity,  Coordinates
Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>1 h 1'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 g 1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 f 1'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 e 1'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 d 1'</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 c 1'</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 b 1'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a 1'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2111'  Along [1,0,0] p2111'  Along [0,1,0] p2111'
\( a^* = a \_p \)  \( b^* = b \_p \)  \( a^* = c \_p \)  \( b^* = a \_p \)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Triclinic

Origin at $\bar{T}'$

Asymmetric unit: $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry Operations:

1. $\bar{T}'$, $0,0,0$
2. $\bar{T}'$, $0,0,0'$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 i 1</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>1 h 1</td>
<td>1/2,1/2,1/2</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>1 g 1</td>
<td>0,1/2,1/2</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>1 f 1</td>
<td>1/2,0,1/2</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>1 e 1</td>
<td>1/2,1/2,0</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>1 d 1</td>
<td>1/2,0,0</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>1 c 1</td>
<td>0,1/2,0</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>1 b 1</td>
<td>0,0,1/2</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>1 a 1</td>
<td>0,0,0</td>
<td>[0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p211  
\(a^* = a_p \quad b^* = b_p\)  
Origin at 0,0,z

Along [1,0,0]  p211  
\(a^* = b_p \quad b^* = c_p\)  
Origin at x,0,0

Along [0,1,0]  p211  
\(a^* = c_p \quad b^* = a_p\)  
Origin at 0,y,0
Triclinic

2.4.7

$P_{2_1}$

Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1; 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

(1) $1$
(1 $| 0,0,0$)
(2) $\bar{1}$ $0,0,0$
(1 $| 0,0,0$)

For $(0,0,1)' +$ set

(1) $t'$ $(0,0,1)$
(1 $| 0,0,1)'$
(2) $\bar{1}'$ $0,0,1/2$
(1 $| 0,0,1)'$
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>(1) (x,y,z) [u,v,w]</td>
</tr>
<tr>
<td>2 h (\bar{1})</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 g (\bar{1})</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 f (\bar{1})</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 e (\bar{1})</td>
<td>1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>2 d (\bar{1})</td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
<tr>
<td>2 c (\bar{1})</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>2 b (\bar{1})</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a (\bar{1})</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] \( p211' \)
  - \( a^* = a_p \)
  - \( b^* = b_p \)
- Along [1,0,0] \( p_{2a}211 \)
  - \( a^* = -c_p \)
  - \( b^* = b_p \)
- Along [0,1,0] \( p_{2a}211 \)
  - \( a^* = c_p \)
  - \( b^* = a_p \)
Monoclinic

P2

3.1.8

P121

Origin on 2

Asymmetric unit 

\[0 < x < 1; \quad 0 < y < 1; \quad 0 < z < \frac{1}{2}\]

Symmetry Operations

\[(1) \quad 1 \quad (2) \quad 0, y, 0\]

\[(1) \quad 0, 0, 0 \quad (2) \quad y, 0, 0\]

Generators selected 

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

\[\begin{array}{c|ccc}
\text{Multiplicity,} & \text{Wyckoff letter,} & \text{Site Symmetry.} \\
\hline
2 & e & 1 & x, y, z [u, v, w] \\
1 & d & 2 & 1/2, y, 1/2 [0, v, 0] \\
1 & c & 2 & 1/2, y, 0 [0, v, 0] \\
1 & b & 2 & y, 1/2 [0, v, 0] \\
1 & a & 2 & y, 0 [0, v, 0] \\
\end{array}\]

Symmetry of Special Projections

Along [0,0,1] \quad p1m'1

\[a^* = a, \quad b^* = b\]

Origin at 0,0,z

Along [1,0,0] \quad p1m1

\[a^* = a, \quad b^* = b\]

Origin at x,0,0

Along [0,1,0] \quad p211

\[a^* = c, \quad b^* = a\]

Origin at 0,y,0

3.1.8 - 1 - 12
**Origin** on 21'

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0
\end{align*}
\]

\[
\begin{align*}
(2) & \quad 0,y,0 \\
(2) & \quad 0,0,0
\end{align*}
\]

For 1' + set

\[
\begin{align*}
(1) & \quad 1' \\
(1) & \quad 0,0,0'
\end{align*}
\]

\[
\begin{align*}
(2) & \quad 0,y,0 \\
(2) & \quad 0,0,0'
\end{align*}
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

Positions
Multiplicty, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>1+</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 e 11'</td>
<td>x,y,z [0,0,0]</td>
<td>(1)</td>
<td>(2)</td>
</tr>
<tr>
<td>1 d 21'</td>
<td>1/2,y,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 c 21'</td>
<td>1/2,y,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 b 21'</td>
<td>0,y,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a 21'</td>
<td>0,y,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] p1m11'  Along [1,0,0] p1m11'  Along [0,1,0] p2111'
\( a^* = a \), \( b^* = b \) \( a^* = -c \), \( b^* = b \) \( a^* = c \), \( b^* = a \)
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
3.3.10 - 1 - 15

P2' 2' Monoclinic

3.2.10 P12'1

Origin on 2'

Asymmetric unit

0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1 (2) 2' 0,y,0
(1 0,0,0) (2 0,0,0)'

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 e 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1)</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>1 d 2'</td>
<td>1/2,y,1/2 [u,0,w]</td>
<td>(2)</td>
<td></td>
</tr>
<tr>
<td>1 c 2'</td>
<td>1/2,y,0 [u,0,w]</td>
<td>(2)</td>
<td></td>
</tr>
<tr>
<td>1 b 2'</td>
<td>0,y,1/2 [u,0,w]</td>
<td>(2)</td>
<td></td>
</tr>
<tr>
<td>1 b 2'</td>
<td>0,y,0 [u,0,w]</td>
<td>(2)</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p1m1

a' = a, b' = b

Origin at 0,0,z

Along [1,0,0] p1m1

a' = -c, b' = b

Origin at x,0,0

Along [0,1,0] p2'11

a' = c, b' = a

Origin at 0,y,0

3.3.10 - 1 - 15
3.4.11 - 1 - 16

P\textsubscript{2\textalpha} 2

3.4.11

P\textsubscript{2\textalpha} 121

Monoclinic

Origin: on 2

Asymmetric unit: 0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/2

Symmetry Operations:

For (0,0,0) +

(1) 1

(1) | 0,0,0

(2) 2 0,y,0

(2) | 0,0,0

For (1,0,0)'

(1) t' (1,0,0)

(1) | 1,0,0'

(2) 2' 1/2,y,0

(2) | 1,0,0'

3.4.11 - 1 - 16
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>(1) ( x,y,z [u,v,w] )</td>
<td>( (0,0,0) + ) ( (1,0,0)' + )</td>
</tr>
<tr>
<td>2 d 2'</td>
<td>1/2, y, 1/2 [u,0,w]</td>
<td>( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>2 c 2'</td>
<td>1/2, y, 0 [u,0,w]</td>
<td>( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>2 b 2</td>
<td>0, y, 1/2 [0,v,0]</td>
<td>( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>2 a 2</td>
<td>0, y, 0 [0,v,0]</td>
<td>( x,y,z [u,v,w] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>( p_{2a} \cdot 1m1 )</th>
<th>Along [1,0,0]</th>
<th>( p_{1m1} )</th>
<th>Along [0,1,0]</th>
<th>( p_{2a} \cdot 211 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a_p ) ( b^* = b )</td>
<td>( a^* = -c_p ) ( b^* = b )</td>
<td>( a^* = -a ) ( b^* = c )</td>
<td>( a^* = -a ) ( b^* = c )</td>
<td>( a^* = -a ) ( b^* = c )</td>
<td>( a^* = -a ) ( b^* = c )</td>
</tr>
<tr>
<td>Origin at 1/2, 0, z</td>
<td>Origin at x, 0, 0</td>
<td>Origin at 0, y, 0</td>
<td>Origin at 0, y, 0</td>
<td>Origin at 0, y, 0</td>
<td>Origin at 0, y, 0</td>
</tr>
</tbody>
</table>
Origin on 2

Asymmetric unit \( 0 \leq x \leq 1; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/2 \)

Symmetry Operations

For \((0,0,0)\) +

(1) \( t \) \((0,0,0)\)  
(1) \( t' \) \((0,1,0)\)  
(1) \( \text{origin} \) on 2

(2) \( t' \) \((0,1,0)\)  
(2) \( t \) \((0,0,0)\)  
(1) \( \text{origin} \) on 2

For \((0,1,0)'\) +

(1) \( t' \) \((0,1,0)\)'  
(2) \( t \) \((0,0,0)\)'  
(2) \( t' \) \((0,0,0)\)'  
(1) \( t \) \((0,0,0)\)  
(1) \( t' \) \((0,1,0)\)  
(1) \( \text{origin} \) on 2

For \((0,1,0)'\) +

Symmetry Operations

Origin on 2
Generators selected \((1); t(1,0,0); t(0,1,0); t(0,0,1); (2)\).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>1</td>
<td>((0,0,0) + (0,1,0))</td>
<td>(x,y,z [u,v,w])</td>
</tr>
<tr>
<td>2 d 2</td>
<td>2</td>
<td>(1/2,y,1/2 [0,v,0])</td>
<td></td>
</tr>
<tr>
<td>2 c 2</td>
<td>2</td>
<td>(1/2,y,0 [0,v,0])</td>
<td></td>
</tr>
<tr>
<td>2 b 2</td>
<td>2</td>
<td>(0,y,1/2 [0,v,0])</td>
<td></td>
</tr>
<tr>
<td>2 a 2</td>
<td>2</td>
<td>(0,y,0 [0,v,0])</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along \([0,0,1]\) \(p_{2b}.1\) \(m'1\)
  - \(a^* = a, b^* = b\)
  - Origin at \(0,0,z\)

- Along \([1,0,0]\) \(p_{2b}.1\) \(m1\)
  - \(a^* = -c, b^* = b\)
  - Origin at \(x,1/2,0\)

- Along \([0,1,0]\) \(p_{2111}'\)
  - \(a^* = c, b^* = a\)
  - Origin at \(0,y,0\)
Origin on 2

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ +

(1) $1$
(1) $0,0,0$

(2) $2$ $0,y,0$
(2) $0,0,0$

For $(1,0,0)' +$

(1) $t'$ $(1,0,0)$
(1) $(1,0,0)'$

(2) $2'$ $1/2,y,0$
(2) $1,0,0'$

$P_c 21'$

3.6.13

$P_c 121$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) ( \bar{x}, y, \bar{z} [\bar{u}, \bar{v}, \bar{w}] )</td>
</tr>
<tr>
<td>2 d 2'</td>
<td>1/2, y, 1/2 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 c 2'</td>
<td>1/2, y, 0 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 2</td>
<td>0, y, 1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2</td>
<td>0, y, 0 [0,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] \( p_1m1 \)
  - \( a^* = a \)
  - \( b^* = b \)
  - Origin at 1/2,0,z
- Along [1,0,0] \( p1m1' \)
  - \( a^* = -c \)
  - \( b^* = b \)
  - Origin at x,0,0
- Along [0,1,0] \( p211' \)
  - \( a^* = c \)
  - \( b^* = a \)
  - Origin at 0,y,0
Origin on 2'\n
Asymmetric unit \(0 \leq x \leq 1; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/2\)

Symmetry Operations

For (0,0,0) +

\(\begin{align*}
1 & \rightarrow 1 \\
0,0,0 & \rightarrow 0,y,0
\end{align*}\)

For (0,1,0)' +

\(\begin{align*}
1' & \rightarrow 1' \\
(0,1,0) & \rightarrow (0,1,0)
\end{align*}\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (0,1,0)’ +</td>
</tr>
<tr>
<td>4 e 1</td>
<td>(1) x,y,z [u,v,w] (2) x,z [u,v,w]</td>
</tr>
<tr>
<td>2 d 2’</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 c 2’</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>2 b 2’</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 a 2’</td>
<td>0,y,0 [u,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p_{2b}1m1</th>
<th>Along [1,0,0] p_{2a}1m1</th>
<th>Along [0,1,0] p_{2111}’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a’ = a         b’ = b</td>
<td>a’ = b         b’ = c</td>
<td>a’ = c         b’ = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
4.1.15 P2₁

Monoclinic

Symmetry Operations

(1) 1
(2) 2 (0,1/2,0) 0,y,0

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

2 a 1 (1) x,y,z [u,v,w] (2) x,y+1/2,z [u,v,w]

Symmetry of Special Projections

Along [0,0,1] p1g’1
a* = a, b* = b
Origin at 0,0,z

Along [1,0,0] p1g’1
a* = -c, b* = b
Origin at x,0,0

Along [0,1,0] p211
a* = c, b* = a
Origin at 0,y,0
### Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2 \]

### Symmetry Operations

**For 1 +**

1. \( (1) \ 1 \)
   - \( (1|0,0,0) \)
2. \( (2) \ 2 \ 0,1/2,0 \)
   - \( 0,y,0 \)

**For 1' +**

1. \( (1) \ 1' \)
   - \( (1|0,0,0)' \)
2. \( (2) \ 2' \ (0,1/2,0) \)
   - \( 0,y,0 \)

### Generators selected

(1): \( (1|0,0,0); \ 1 \)
(2): \( (1|0,0,0); \ 1' \)

### Positions

**Multiplicity, Wyckoff letter, Site Symmetry.**

1+ 1'

1. \( a \)
   - \( 0 \leq x \leq 1; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/2 \)
   - \( (1) \ x,y,z \ [0,0,0] \)
   - \( (2) \ x,y+1/2,z \ [0,0,0] \)

### Symmetry of Special Projections

**Along [0,0,1]** \( p1g11' \)

\( a^* = a \)
\( b^* = b \)

**Along [1,0,0]** \( p1g11' \)

\( a^* = -c \)
\( b^* = b \)

**Along [0,1,0]** \( p2111' \)

\( a^* = c \)
\( b^* = a \)
**Origin** on $2'_1$

**Asymmetric unit**
$$0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$$

**Symmetry Operations**

(1) 1
(2) 2' $(0,1/2,0)$ 0,y,0

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

2 a 1

(1) $x,y,z$ [u,v,w]
(2) $x,y+1/2,z$ [u,$\bar{v}$,w]

**Symmetry of Special Projections**

Along [0,0,1] p1g1

$a^* = a$, $b^* = b$

Origin at 0,0,z

Along [1,0,0] p1g1

$a^* = -c$, $b^* = b$

Origin at x,0,0

Along [0,1,0] p2'11

$a^* = c$, $b^* = a$

Origin at 0,y,0
4.4.18 - 1 - 27

**Origin** on 2₁

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For (0,0,0) +

1. \((1) \quad \begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix} \)
   \((2) \quad \begin{pmatrix} 2 \quad (0,1/2,0) \\ 0,y,0 \end{pmatrix} \)

For \((1,0,0)^*\) +

1. \((1) \quad t(1,0,0) \)
   \((2) \quad t(0,1,0) \)
   \((3) \quad t(0,0,1) \)
   \((4) \quad t(0,1,0) \)

**Generators selected**

\((1); t(1,0,0)^*; t(0,1,0); t(0,0,1); (2).\)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0) + (1,0,0)^* +)</td>
<td></td>
</tr>
</tbody>
</table>

\[ \begin{align*} 
4 & \quad \begin{pmatrix} a \quad 1 \end{pmatrix} \quad \begin{pmatrix} (1) \quad x,y, z [u,v,w] \end{pmatrix} \quad \begin{pmatrix} (2) \quad x,y+1/2, z [u,v,w] \end{pmatrix} 
\end{align*} \]

**Symmetry of Special Projections**

Along \([0,0,1]\) \(p_{2a-1g1}\)

\[ a^* = a, \quad b^* = b \]

Origin at \(1/2,0,z\)

Along \([1,0,0]\) \(p1g1\)

\[ a^* = -c, \quad b^* = b \]

Origin at \(x,0,0\)

Along \([0,1,0]\) \(p_{2a21}\)

\[ a^* = -a, \quad b^* = c \]

Origin at \(0,y,0\)
5.1.19 - 1 - 28

C2

2

Monoclinic

5.1.19 C121

Origin on 2

Asymmetric unit

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1 \]

Symmetry Operations

For \((0,0,0) +\) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 0,y,0 \\
(1^*0,0,0) & \quad (2^*y,0,0) \\
\end{align*}
\]

For \((1/2,1/2,0) +\) set

\[
\begin{align*}
(1) & \quad t(1/2,1/2,0) \\
(2) & \quad (0,1/2,0) 1/4,y,0 \\
(1^*1/2,1/2,0) & \quad (2^*1/2,1/2,0) \\
\end{align*}
\]
Continued

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).

**Positions**  

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>c</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>b</td>
<td>4 x,y,z [u,v,w] (2) x̄,ȳ,z̄ [ū,v̄,w̄]</td>
</tr>
<tr>
<td>a</td>
<td>2 0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>2 0,y,0 [0,v,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**  

<table>
<thead>
<tr>
<th>Origin</th>
<th>Along [0,0,1] c1m'1</th>
<th>Along [1,0,0] p1m'1</th>
<th>Along [0,1,0] p211</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -c</td>
<td>a* = c</td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = b/2</td>
<td>b* = b/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
C21' 21' Monoclinic

5.2.20

C1211'

Origin on 21'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,y,0 \\
\text{(1)} & \quad (0,0,0) \\
\text{(2)} & \quad (0,0,0)
\end{align*}
\]

For \((1/2,1/2,0)\) + set

\[
\begin{align*}
(1) & \quad t \\
(2) & \quad 2 \quad 0,1/2,0 \\
\text{(1)} & \quad 1/2,1/2,0 \\
\text{(2)} & \quad 1/2,1/2,0
\end{align*}
\]

For \((0,0,0)\)' + set

\[
\begin{align*}
(1) & \quad 1' \\
(2) & \quad 2' \quad 0,y,0 \\
\text{(1)} & \quad (0,0,0)' \\
\text{(2)} & \quad (0,0,0)'
\end{align*}
\]

For \((1/2,1/2,0)\)' + set

\[
\begin{align*}
(1) & \quad t' \\
(2) & \quad 2' \quad 0,1/2,0 \\
\text{(1)} & \quad 1/2,1/2,0' \\
\text{(2)} & \quad 1/2,1/2,0'
\end{align*}
\]
Continued

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 11'</td>
<td>(1) x, y, z</td>
<td>[0,0,0]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z</td>
<td></td>
<td>(1/2,1/2,0) +</td>
</tr>
</tbody>
</table>

| 2 b 21'      | 0, y, 1/2      | [0,0,0]       |
| 2 a 21'      | 0, y, 0        | [0,0,0]       |

**Symmetry of Special Projections**

- Along [0,0,1] c1m11'
  - Origin at 0,0,z
  - \( a^* = a, b^* = b \)

- Along [1,0,0] p1m11'
  - Origin at x,0,0
  - \( a^* = -c, b^* = b/2 \)

- Along [0,1,0] p2111'
  - Origin at 0,y,0
  - \( a^* = c, b^* = a/2 \)
C2’ 2’

5.3.21 C12’1

Concrete

Origin on 2’

Asymmetric unit 
0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2’ 0,y,0
(2,|0,0,0)’

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1|1/2,1/2,0)

(2) 2’ (0,1/2,0) 1/4,y,0
(2,|1/2,1/2,0)’

5.3.21 - 1 - 32
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
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<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>2 b 2'</td>
<td>0,y,1/2</td>
<td>[u,0,w]</td>
<td>(1/2,1,2,0)</td>
</tr>
<tr>
<td>2 a 2'</td>
<td>0,y,0</td>
<td>[u,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c1m1

a* = a, b* = b

Origin at 0,0,z

Along [1,0,0] p1m1

a* = -c, b* = b/2

Origin at x,0,0

Along [0,1,0] p2'11

a* = c, b* = a/2

Origin at 0,y,0
Origin on 2

Asymmetric unit  
\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1\]

Symmetry Operations

For \((0,0,0)\) + set

1. \((1)\)  
   \((1\ 0,0,0)\)  
   \((2)\ 0,y,0\)

2. \((2\ 0,0,0)\)

For \((1/2,1/2,0)\) + set

1. \((1)\ t\ (1/2,1/2,0)\)  
   \((1\ 1/2,1/2,0)\)

2. \((2\ 0,1/2,0)\)  
   \((2\ 1/4,y,0)\)

   \((2\ 1/2,1/2,0)\)

For \((0,0,1)'\) + set

1. \((1)\ t'\ (0,0,1)\)  
   \((1\ 0,0,1)'\)

2. \((2\ 0,y,1/2)\)  
   \((2\ 0,0,1)'\)

For \((1/2,1/2,1)'\) + set

1. \((1)\ t'\ (1/2,1/2,1)\)  
   \((1\ 1/2,1/2,1)'\)

2. \((2\ 0,1/2,0)\)  
   \((2\ 1/4,y,1/2)\)

   \((2\ 1/2,1/2,1)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) (\bar{x},y,\bar{z} [u,v,\bar{w}])</td>
</tr>
<tr>
<td>4 b 2'</td>
<td>0,y,1/2 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 a 2</td>
<td>0,y,0 [0,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  \(c1m1\)'  
\(a^* = a\)
\(b^* = b\)
Origin at 0,0,z

Along [1,0,0]  \(p_{2\alpha}1\text{m}1\)  
\(a^* = -c\)
\(b^* = b/2\)
Origin at 0,0,0

Along [0,1,0]  \(p_{2\alpha}2\text{11}\)  
\(a^* = c\)
\(b^* = a/2\)
Origin at 0,y,0
**Symmetry Operations**

For \((0,0,0)\) set

(1) \(1\)

\((1|0,0,0)\)

(2) \(2\) \(0,y,0\)

\((2|0,0,0)\)

For \((1/2,1/2,0)\) set

(1) \(t\) \((1/2,1/2,0)\)

\((1|1/2,1/2,0)\)

(2) \(2^t\) \((0,1/2,0)\) \(1/4,y,0\)

\((2,1/2,1/2,0)\)

**Asymmetric unit**

\(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)
Generators selected: \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2)\).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 b 2</td>
<td>0,y,1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2</td>
<td>0,y,0 [0,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \(c_p1m'1\)
\(a^* = a\), \(b^* = b\)
Origin at 0,0,z

Along \([1,0,0]\) \(p_{2b1m'1}\)
\(a^* = -c\), \(b^* = b/2\)
Origin at x,0,0

Along \([0,1,0]\) \(p_{2a211}\)
\(a^* = c\), \(b^* = a/2\)
Origin at 0,y,0
**Origin** on 2'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. 1
   - \((1|0,0,0)\)
   - \((2|0,0,0)\)

For \((1/2,1/2,0)\)' + set

1. \(t'\) \((1/2,1/2,0)\)
   - \((1|1/2,1/2,0)\)
   - \((2|1/2,1/2,0)\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>c 1</td>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>b 2'</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>a 2'</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>a 2'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c, 1m1

Along [1,0,0] p, 1m1

Along [0,1,0] p, 211

Origin at 0,0,z

Origin at x,0,0

Origin at 1/4,y,0
Pm  m  Monoclinic
6.1.25  P1m1

Asymmetric unit  0 ≤ x ≤ 1; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1  (2) m  x,0,z
(1|0,0,0)     (m|0,0,0)

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>a</td>
<td>m</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>c</td>
<td>m</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>m</td>
<td>x,0,z [0,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p1m1  Along [1,0,0]  p1m1  Along [0,1,0]  p11'
a* = -b  b* = a  a* = b  b* = c  a* = c  b* = a  Origin at 0,0,z
Origin at x,0,0  Origin at 0,y,0
6.2.26 - 1 - 41

**Monoclinic**

**Origin** on \( m_1' \)

**Asymmetric unit**

\[
0 < x < 1; \quad 0 < y < 1/2; \quad 0 < z < 1
\]

**Symmetry Operations**

For 1 + set

1. \((1)|0,0,0\)
2. \((2) m_1 x,0,z (m_1 y,0,0)\)

For 1' + set

1. \((1)'|0,0,0\)
2. \((2) m_1' x,0,z (m_1 y,0,0)'\)
Generators selected \[(1); \tau(1,0,0); \tau(0,1,0); \tau(0,0,1); (2); 1'.\]

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 11'</td>
<td>(1) x, y, z [0, 0, 0]</td>
<td></td>
<td>(2) x, \bar{y}, z [0, 0, 0]</td>
</tr>
<tr>
<td>1 b m1'</td>
<td>x, 1/2, z [0, 0, 0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a m1'</td>
<td>x, 0, z [0, 0, 0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0, 0, 1] \(p1m11'\) \(a^* = -b\) \(b^* = a_p\) Origin at 0, 0, z
Along [1, 0, 0] \(p1m11'\) \(a^* = b\) \(b^* = c_p\) Origin at x, 0, 0
Along [0, 1, 0] \(p11'\) \(a^* = c\) \(b^* = a\) Origin at 0, y, 0
Pm' m' Monoclinic
6.3.27 P1m'1

Origin on m'

Asymmetric unit

0 < x < 1; 0 < y < 1/2; 0 < z < 1

Symmetry Operations

(1) 1 (2) m' x,0,z
(1 | 0,0,0) (m' | 0,0,0)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>1 b m'</td>
<td>x,1/2,z [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>1 a m'</td>
<td>x,0,z [u,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p1m'1

\( a^* = -b \quad b^* = a_p \)

Origin at 0,0,z

Along [1,0,0] p1m'1

\( a^* = b \quad b^* = c_p \)

Origin at x,0,0

Along [0,1,0] p1

\( a^* = c \quad b^* = a \)

Origin at 0,y,0
Origin on m

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

- \((1)\) 1
- \((1|0,0,0)\)
- \((m|0,0,0)\)

For \((1,0,0)\)' + set

- \((1)\) t' (1,0,0)
- \((1|1,0,0)\)'
- \((m|1,0,0)\)'
- \((a'|1,0,0)\) x,0,z
Continued

6.4.28

**P_{2_1}m**

**Generators selected**
(1); t(1,0,0)'; t(0,1,0); t(0,0,1); (2).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 b m</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>2 a m</td>
<td>x,0,z [0,v,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_{2_1}m1</th>
<th>Along [1,0,0]</th>
<th>p1m1'</th>
<th>Along [0,1,0]</th>
<th>p11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>a* = b</td>
<td>a* = c</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>b* = a_p</td>
<td>b* = c_p</td>
<td>b* = a</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.5.29

**M1'**

**P2bm m1'**

**Monoclinic**

**Origin** on m

**Asymmetric unit**

\[0 < x < 1; \quad 0 < y < 1/2; \quad 0 < z < 1\]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \(1\)
   
   \((0,0,0)\)
   
   \((m_y 0,0,0)\)

For \((0,1,0)' + \text{set}\)

1. \(t'\)
   
   \((0,1,0)'\)
   
   \((m_y 0,1,0)'\)

1. \(m'\)
   
   \((0,1,0)\)
   
   \((m_y 0,1,0)\)
Generators selected \( (1); \ t(1,0,0'); \ t(0,1,0'); \ t(0,0,1); \ (2). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) ( x,y,z \ [u,v,w] )</td>
</tr>
<tr>
<td>2 b m'</td>
<td>(2) ( x,y,z \ [u,v,w] )</td>
</tr>
<tr>
<td>2 a m</td>
<td>( x,1/2,z \ [u,0,w] )</td>
</tr>
<tr>
<td></td>
<td>( x,0,z \ [0,v,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>( p_{2a\cdot1m1} )</th>
<th>Along [1,0,0]</th>
<th>( p_{2a\cdot1m1} )</th>
<th>Along [0,1,0]</th>
<th>( p11' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = -b )</td>
<td>( b^* = a_p )</td>
<td>( a^* = b )</td>
<td>( b^* = c_p )</td>
<td>( a^* = c )</td>
<td>( b^* = a )</td>
</tr>
<tr>
<td>Origin at ( 0,0,z )</td>
<td>Origin at ( x,0,0 )</td>
<td>Origin at ( 0,y,0 )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
PCm m1' Monoclinic
6.6.30 Pc1m1

Origin on m

Asymmetric unit
0 \leq x \leq 1; 0 \leq y \leq 1/2; 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1|0,0,0)
   (m_y|0,0,0)

(2) m x,0,z

For (1,0,0)' + set

(1) t' (1,0,0)
   (1|1,0,0)'
   (m_y|1,0,0)'

(2) a' (1,0,0) x,0,z

6.6.30 - 1 - 48
Continued

Generators selected  (1); t(1,0,0)'; t(0,1,0)'; t(0,0,1); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (1,0,0)' +

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>2 b m'</td>
<td>x,1/2,z [u,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a m</td>
<td>x,0,z [0,v,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p₃1m1  Along [1,0,0]  p1m11'  Along [0,1,0]  p11'

\( a^* = -b \quad b^* = a_p \quad a^* = b \quad b^* = c_p \quad a^* = c \quad b^* = a \)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on m

Asymmetric unit

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\]

Symmetry Operations

For \((0,0,0)\) + set

\[(1) \ 1 \quad (2) m' \ x,0,z \quad (m' y,0,0)'

For \((0,0,1)\)' + set

\[(1) t' \ (0,0,1) \quad (2) c (0,0,1) \ x,0,z \quad (m' y,0,0,1)\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(0,0,1)' +</td>
<td>x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4 c 1</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2)</td>
<td>x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2 b m</th>
<th>x,1/2,z [0,v,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 a m'</td>
<td>x,0,z [u,0,v]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1]  
  \( p1m1' \)  
  \( a^* = b \) \( b^* = a \)  
  Origin at 0,0,z

- Along [1,0,0]  
  \( p_{2b}1m'1 \)  
  \( a^* = b \) \( b^* = c \)  
  Origin at x,0,0

- Along [0,1,0]  
  \( p11' \)  
  \( a^* = c \) \( b^* = a \)  
  Origin at 0,y,0
Pc m Monoclinic
7.1.32 P1c1

Origin on glide plane $c$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

(1) 1
(1) 0,0,0
(1 0,0,0)

(2) c $(0,0,1/2)$ $x,0,z$
(2) $m_{1/2}$ $(0,0,1/2)$

Generators selected (1); $t(1,0,0); t(0,1,0); t(0,0,1); (2)$.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 a 1</td>
<td>$x,y,z [u,v,w]$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$(2) \bar{x},y,z+1/2 [\bar{u},v,w]$</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along $[0,0,1]$ $p1m1$
$\mathbf{a}^* = -\mathbf{b}$ $\mathbf{b}^* = \mathbf{a}_p$
Origin at $0,0,z$

Along $[1,0,0]$ $p1g1$
$\mathbf{a}^* = \mathbf{b}$ $\mathbf{b}^* = \mathbf{c}_p$
Origin at $x,0,0$

Along $[0,1,0]$ $\mathbf{p}_{2\perp 1}$
$\mathbf{a}^* = \mathbf{c}/2$ $\mathbf{b}^* = \mathbf{a}$
Origin at $0,y,0$
Origin on glide plane \( c1' \)

Asymmetric unit \( 0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \( 1 + \) set

(1) \( 1 \)

(1') \( 1' \)

(2) \( c \) \( (0,0,1/2) \) \( x,0,z \)

(2') \( c' \) \( (0,0,1/2) \) \( x,0,z \)

For \( 1' + \) set

(1) \( 1' \)

(1') \( 1' \)

(2) \( c' \) \( (0,0,1/2) \) \( x,0,z \)

(2') \( c \) \( (0,0,1/2) \) \( x,0,z \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>1 + 1' +</td>
</tr>
<tr>
<td>2 a 11'</td>
<td>(1) x,y,z [0,0,0] (2) x, y,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p1m11'  Along [1,0,0] p1g11'  Along [0,1,0] p11'

\[
\begin{align*}
\mathbf{a}^* &= -\mathbf{b} & \mathbf{b}^* &= \mathbf{a}_p \\
\mathbf{a}^* &= \mathbf{b} & \mathbf{b}^* &= \mathbf{c}_p \\
\mathbf{a}^* &= \mathbf{c}/2 & \mathbf{b}^* &= \mathbf{a}
\end{align*}
\]

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on glide plane $c'$

Asymmetric unit

$$0 < x < 1; \quad 0 < y < 1/2; \quad 0 < z < 1$$

Symmetry Operations

(1) $1$

(2) $c' \quad (0,0,1/2) \quad x,0,z$

Generators selected

(1); $t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ (2)$. 

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 a 1 (1) $x,y,z \ [u,v,w]$ (2) $x$, $y$, $z+1/2 \ [u$, $v$, $w]$</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] $p1m'1$  
Along [1,0,0] $p1g'1$  
Along [0,1,0] $p1$

$a^* = -b$  
$b^* = a$

Origin at 0,0,z  
 Origin at x,0,0  
 Origin at 0,y,0
**P2\(\text{ac}m1\)’ Monoclinic**

**Origin** on glide plane \(c\)

**Asymmetric unit** 
\[0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \((1) 1\)
   1. \((1|0,0,0)\)
   2. \((2) c (0,0,1/2) x,0,z\)
   3. \((m_y|0,0,1/2)\)

For \((1,0,0)\)' + set

1. \((1) t' (1,0,0)\)
   1. \((1|1,0,0)\)
   2. \((2) n' (1,0,1/2) x,0,z\)
   3. \((m_y|1,0,1/2)'\)

**Generators selected**

(1); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); (2).

**Positions**

**Multiplicities, Wyckoff letters, Site Symmetry.**

\[
\begin{align*}
4 & \quad a \quad 1 \\
(0,0,0) + & \quad (1,0,0)' + \\
(1) & \quad x,y,z [u,v,w] \\
(2) & \quad x, y, z+1/2 [u,v,w]
\end{align*}
\]

**Symmetry of Special Projections**

Along \([0,0,1]\) \(p_{2\text{ac}}.1m1\)

\[
\begin{align*}
a^* &= -b & b^* &= a_p \\
\text{Origin at } 0,0,z
\end{align*}
\]

Along \([1,0,0]\) \(p1g11'\)

\[
\begin{align*}
a^* &= b & b^* &= c_p \\
\text{Origin at } x,0,0
\end{align*}
\]

Along \([0,1,0]\) \(p_{2\text{ac}}.1\)

\[
\begin{align*}
a^* &= -a & b^* &= c/2 \\
\text{Origin at } 0,y,0
\end{align*}
\]
Origin on glide plane c

Asymmetric unit  
0 ≤ x ≤ 1; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations
For (0,0,0) + set

(1) 1  
(1|0,0,0)  
(2) c  (0,0,1/2)   x,0,z  
(m|0,0,1/2)

For (0,1,0)'+ set

(1) t' (0,1,0)  
(1|0,1,0)  
(2) c' (0,0,1/2)   x,1/2,z  
(m|0,1,1/2)'

Generators selected  
(1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

4 a 1  
(1) x,y,z [u,v,w]  
(2) x, y,z+1/2 [u,v,w]

Symmetry of Special Projections

Along [0,0,1]  

p_{2a}-1m1  

a^* = -b  \quad b^* = a_p  
Origin at 0,0,z

Along [1,0,0]  

p_{2a}-1g1  

a^* = b  \quad b^* = c_o  
Origin at x,0,0

Along [0,1,0]  

p11'  

a^* = c/2  \quad b^* = a  
Origin at 0,y,0

7.5.36 - 1 - 57
Origin on glide plane  $c$

**Asymmetric unit**

$0 \leq x \leq 1$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$

**Symmetry Operations**

For $(0,0,0)$ + set

1. $1$
   - $(1) 1$
   - $(1|0,0,0)$
   - $(0,0,1/2)$ $x,0,z$
   - $(m_y,0,0,1/2)$

For $(1,0,0)' + set$

1. $t'$ $(1,0,0)$
   - $(1|1,0,0)'$
   - $(1,0,1/2)$ $x,0,z$
   - $(m_y,1,0,1/2)'$

**Generators selected**

(1); $t(1,0,0)'$; $t(0,1,0)'$; $t(0,0,1)$; (2).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 $a$ 1</td>
<td>(1) $x,y,z [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>(2) $x, y,z+1/2 [\bar{u},v,\bar{w}]$</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1]  $p_c1m1$
  - $a^* = -b$  $b^* = a_p$
  - Origin at 0,0,z

- Along [1,0,0]  $p1g11'$
  - $a^* = b$  $b^* = c_o$
  - Origin at x,0,0

- Along [0,1,0]  $p11'$
  - $a^* = a$  $b^* = c/2$
  - Origin at 0,y,0
Cm m Monoclinic

8.1.38 C1m1

Origin on mirror plane m

Asymmetric unit

0 ≤ x ≤ 1;
0 ≤ y ≤ 1/4;
0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) m x,0,z
(m | 0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)

(2) a (1/2,0,0) x,1/4,z
(m | 1/2,1/2,0)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).

Positions

Multiplicaty,
Wyckoff letter,
Site Symmetry.

(0,0,0) +

(1/2,1/2,0) +

4 b 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w]

2 a m x,0,z [0,v,0]

Symmetry of Special Projections

Along [0,0,1] c1m1

a* = -b b* = a_p
Origin at 0,0,z

Along [1,0,0] p1m1

a* = b/2 b* = c_p
Origin at x,0,0

Along [0,1,0] p11'

a* = c b* = a/2
Origin at 0,y,0

8.1.38 - 1 - 59
Origin on mirror plane $m1'$

Asymmetric unit

$0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

(1) $1$

(1) $t (1/2,1/2,0)$

(1) $t' (1/2,1/2,0)$

(1) $1'$

(1) $t' (1/2,1/2,0)$

(1) $1$ (0,0,0)

(1) $1/2,1/2,0)$

(1) $1/2,1/2,0)$

(1) $0,0,0)$

(1) $0,0,0)'$

(1) $0,0,0)'$

(1) $0,0,0)'$

(1) $0,0,0)'$

(1) $0,0,0)'$

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(1) $0,0,0)'$

(1) $0,0,0)'$
Generators selected  
(1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2): 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' +</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>4 b 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0]</td>
<td>(0,0,0)' + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>2 a m1' x,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c1m11'  
\( a^* = -b \quad b^* = a_p \)  
Origin at 0,0,z

Along [1,0,0] p1m11'  
\( a^* = b/2 \quad b^* = c_p \)  
Origin at x,0,0

Along [0,1,0] p11'  
\( a^* = c \quad b^* = a/2 \)  
Origin at 0,y,0
Cm’ m’ Monoclinic

\[ 8.3.40 \quad C1m’1 \]

Origin on mirror plane \( m’ \)

Asymmetric unit

\[
0 < x < 1; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1
\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad \mathbf{1} \\
(1) & \quad (0,0,0) \\
(2) & \quad m’ \quad x,0,z \\
& \quad (m_{\overline{1}} \overline{0},0,0)'
\end{align*}
\]

For \((1/2,1/2,0) + \) set

\[
\begin{align*}
(1) & \quad t \quad (1/2,1/2,0) \\
(1) & \quad (1/2,1/2,0) \\
(2) & \quad a’ \quad (1/2,0,0) \quad x,1/4,z \\
& \quad (m_{\overline{1}} \overline{1/2},1/2,0)'
\end{align*}
\]

Generators selected

\((1); \quad t(1,0,0); \quad t(0,1,0); \quad t(0,0,1); \quad t(1/2,1/2,0); \quad (2).\)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4 \quad b' \quad 1 )</td>
<td>(x,y,z \ [u,v,w])</td>
<td>(x,0,z \ [u,0,w])</td>
<td>((0,0,0) + )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1] \quad c1m’1 \)

\( a'^* = -b \quad b'^* = a_p \)

Origin at \(0,0,z \)

Along \([1,0,0] \quad p1m’1 \)

\( a'^* = b/2 \quad b'^* = c_p \)

Origin at \(x,0,0 \)

Along \([0,1,0] \quad p1 \)

\( a'^* = c \quad b'^* = a/2 \)

Origin at \(0,y,0 \)
Origin on mirror plane m

Asymmetric unit
\[ 0 \leq x \leq 1; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

**For \((0,0,0) + set\)**

1. \(1\)
   - \((1,0,0,0)\)
   - \((m,0,0,0)\)

2. \(m\) \(x,0,z\)
   - \((m,0,0,0)\)

**For \((1/2,1/2,0) + set\)**

1. \(t\) \((1/2,1/2,0)\)
   - \((1/2,1/2,0,0)\)
   - \((m,1/2,1/2,0,0)\)

2. \(a\) \((1/2,0,0)\) \(x,1/4,z\)
   - \((m,1/2,0,0)\)

**For \((0,0,1)' + set\)**

1. \(t'\) \((0,0,1)\)
   - \((0,0,1)'\)
   - \((m,0,0,1)'\)

2. \(c'\) \((0,0,1)\) \(x,0,z\)
   - \((m,0,0,1)'\)

**For \((1/2,1/2,1)' + set\)**

1. \(t'\) \((1/2,1/2,1)\)
   - \((1/2,1/2,1,0)\)
   - \((m,1/2,1/2,1,0)\)

2. \(n'\) \((1/2,0,1)\) \(x,1/4,z\)
   - \((m,1/2,0,1)'\)
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1'); t(1/2,1/2,0); (2). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) ( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>4 a m</td>
<td>(2) ( x,y,\bar{z} [\bar{u},v,w] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = -b )</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>( p_{1b}1m1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = b/2 )</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>( p11' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = c )</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
8.5.42 - 1 - 65

**CPm m1'**

**Monoclinic**

**Origin**

on mirror plane m

**Asymmetric unit**

$0 \leq x \leq 1$; $0 \leq y \leq 1/4$; $0 \leq z \leq 1$

**Symmetry Operations**

For (0,0,0) + set

(1) $1$

(1) $0,0,0$

(2) m $x,0,z$

(2) $m_{y}0,0,0$

For (1/2,1/2,0)' + set

(1) $t'$ (1/2,1/2,0)

(1) $1/2,1/2,0$

(2) a' (1/2,0,0) $x,1/4,z$

(2) $m_{y}1/2,1/2,0$

**Generators selected**

(1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(1/2,1/2,0)'$; (2).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) +

(1/2,1/2,0)'

4 b 1

(1) $x,y,z$ [$u,v,w$]

(2) $x,y,z$ [$\bar{u},v,\bar{w}$]

2 a m

$x,0,z$ [$0,v,0$]

**Symmetry of Special Projections**

Along [0,0,1] $c_p1m1$

$\mathbf{a}^* = -b$ $\mathbf{b}^* = a_p$

Origin at 0,0,0

Along [1,0,0] $p_{2a}1m1$

$\mathbf{a}^* = \mathbf{b}/2$ $\mathbf{b}^* = \mathbf{c}_p$

Origin at x,0,0

Along [0,1,0] $p11'$

$\mathbf{a}^* = \mathbf{c}$ $\mathbf{b}^* = \mathbf{a}/2$

Origin at 0,y,0
**C2cm' m1'**

8.6.43

**Monoclinic**

**Origin**
on mirror plane m'

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y < 1/4; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \((1)\ 1\)\n   
   \((1)\ 0,0,0\)
   
   \((2)\ m'\ x,0,z\)\n   
   \((m_y|0,0,0)')\n
For \((1/2,1/2,0) + \) set

1. \((1)\ t\)\n   
   \((1)\ 1/2,1/2,0\)
   
   \((2)\ a'\ (1/2,0,0)\)\n   
   \((1/2,0,0)')\n
For \((0,0,1) + \) set

1. \((1)\ t'\)\n   
   \((1)\ 0,0,1\)
   
   \((2)\ c\ (0,0,1)\)\n   
   \((0,0,1)')\n
For \((1/2,1/2,1) + \) set

1. \((1)\ t'\)\n   
   \((1)\ 1/2,1/2,1\)
   
   \((2)\ n\ (1/2,0,1)\)\n   
   \((1/2,0,1)')\n
8.6.43 - 1 - 66
Continued

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 a m'</td>
<td>x,0,z [u,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = -b)</td>
<td>(b^* = a_p)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>(p_{2a'1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = b/2)</td>
<td>(b^* = c_p)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>(p_{2b'1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = c)</td>
<td>(b^* = a/2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Origin at x,0,0</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Origin at 0,y,0</th>
</tr>
</thead>
</table>
**CPm' m'**  
**Monoclinic**  
8.7.44  
**C_p1m'1**

**Origin**  
on mirror plane m'

**Asymmetric unit**  
0 ≤ x ≤ 1;  0 ≤ y ≤ 1/4;  0 ≤ z ≤ 1

**Symmetry Operations**

For (0,0,0) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>m'</td>
<td>x,0,z</td>
</tr>
<tr>
<td>2</td>
<td>m'</td>
<td>(m_y,0,0)</td>
</tr>
</tbody>
</table>

For (1/2,1/2,0)' + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>t(1/2,1/2,0)'</td>
<td>(m_y,1/2,1/2,0)</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>x,1/4,z</td>
</tr>
</tbody>
</table>

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 b 1</td>
<td>x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>2 a m'</td>
<td>x,0,z [u,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Origin</th>
<th>a* = -b  b* = a_p</th>
<th>Along [0,0,1]  C_p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,0,z</td>
<td>a* = -b/2  b* = c_p</td>
<td>Along [1,0,0] p_{2a'}1m1</td>
</tr>
<tr>
<td>0,y,0</td>
<td>a* = -a/2  b* = c</td>
<td>Along [0,1,0] p_{2a'}1</td>
</tr>
</tbody>
</table>

8.7.44 - 1 - 68
Origin on glide plane c

Asymmetric unit

\[ 0 < x < 1; \quad 0 < y < 1/4; \quad 0 < z < 1 \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad c \quad (0,0,1/2) \quad x,0,z \\
(1^*_{0,0,0}) & \quad (m_y,0,0,1/2)
\end{align*}
\]

For \((1/2,1/2,0) + \) set

\[
\begin{align*}
(1) & \quad t \quad (1/2,1/2,0) \quad x,1/4,z \\
(2) & \quad n \quad (1/2,0,1/2) \quad x,1/4,z \\
(1^*_{1/2,1/2,0}) & \quad (m_y,1/2,1/2,1/2)
\end{align*}
\]

Generators selected

\((1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).\)

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

\[
\begin{align*}
(0,0,0) + & \quad (1/2,1/2,0) + \\
4 \quad a \quad 1 & \quad (1) \quad x,y,z [u,v,w] \\
& \quad (2) \quad x,y,z+1/2 [u,v,w]
\end{align*}
\]

Symmetry of Special Projections

Along \([0,0,1]\) \quad c1m1

\[
a^* = -b \quad b^* = a_p \quad \text{Origin at } 0,0,z
\]

Along \([1,0,0]\) \quad p1g1

\[
a^* = b/2 \quad b^* = c_p \quad \text{Origin at } x,0,0
\]

Along \([0,1,0]\) \quad P_{21}1

\[
a^* = c/2 \quad b^* = a/2 \quad \text{Origin at } 0,y,0
\]

9.1.45 - 1 - 69
Origin on glide plane c1'

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1') & \quad 1'
\end{align*}
\]

\[
\begin{align*}
(2) & \quad c \quad (0,0,1/2) \\
(m) & \quad (0,0,1/2)
\end{align*}
\]

For \((1/2,1/2,0)\) + set

\[
\begin{align*}
(1) & \quad t \quad (1/2,1/2,0) \\
(1') & \quad t'
\end{align*}
\]

\[
\begin{align*}
(2) & \quad n \quad (1/2,0,1/2) \\
(m) & \quad (1/2,1/2,1/2)
\end{align*}
\]

For \((0,0,0)'\) + set

\[
\begin{align*}
(1) & \quad 1' \\
(1') & \quad 1'
\end{align*}
\]

\[
\begin{align*}
(2) & \quad c' \quad (0,0,1/2) \\
(m) & \quad (0,0,1/2)'
\end{align*}
\]

For \((1/2,1/2,0)'\) + set

\[
\begin{align*}
(1) & \quad t' \quad (1/2,1/2,0) \\
(1') & \quad t'
\end{align*}
\]

\[
\begin{align*}
(2) & \quad n' \quad (1/2,0,1/2) \\
(m) & \quad (1/2,1/2,1/2)'
\end{align*}
\]
Generators selected:

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' +</td>
<td>x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 a 11' (1) x,y,z [0,0,0]</td>
<td>x,y,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c1m11'

\[ \mathbf{a}^* = -\mathbf{b}, \quad \mathbf{b}^* = \mathbf{a}_p \]

Origin at 0,0,z

Along [1,0,0] p1g11'

\[ \mathbf{a}^* = \mathbf{b}/2, \quad \mathbf{b}^* = \mathbf{c}_p \]

Origin at x,0,0

Along [0,1,0] p11'

\[ \mathbf{a}^* = \mathbf{c}/2, \quad \mathbf{b}^* = \mathbf{a}/2 \]

Origin at 0,y,0
**Cc' m' Monoclinic**

9.3.47  C1c'1

**Origin** on glide plane c'

**Asymmetric unit**

\[ 0 < x < 1; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \(1\)
   
   \[ (1) 1 \]
   
   \[ (1|0,0,0) \]

2. \(c'\)
   
   \[ (2) c' (0,0,1/2) \]
   
   \[ x,0,z \]

   \[ (m_y|0,0,1/2)' \]

For \((1/2,1/2,0) + \) set

1. \(t\)
   
   \[ (1) t (1/2,1/2,0) \]
   
   \[ x,1/4,z \]

   \[ (1/2,1/2,1/2)' \]

2. \(n'\)
   
   \[ (2) n' (1/2,0,1/2) \]
   
   \[ x,1/4,z \]

   \[ (m_y|1/2,1/2,1/2)' \]

**Generators selected**

1. \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2).\)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0) + )</td>
<td>((1/2,1/2,0) + )</td>
</tr>
</tbody>
</table>

| 4 a 1 | \(x,y,z [u,v,w] \)
| 2 x, y, z+1/2 [u, v, w] |

**Symmetry of Special Projections**

Along \([0,0,1] \) \(c1m'1 \)

\[ a^* = -b \quad b^* = a_p \]

Origin at 0,0,z

Along \([1,0,0] \) \(p1g'1 \)

\[ a^* = b/2 \quad b^* = c_p \]

Origin at x,0,0

Along \([0,1,0] \) \(p1 \)

\[ a^* = c/2 \quad b^* = a/2 \]

Origin at 0,y,0
CPm1' Monoclinic
9.4.48 C \text{P}1c1

Origin on glide plane c

Asymmetric unit
0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1

Symmetry Operations
For (0,0,0) + set

(1) \text{t} (0,0,0) (2) c (0,0,1/2) x,0,z

(m, 0,0,1/2)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0) (2) n' (1/2,0,1/2) x,1/4,z

(m, 1/2,1/2,1/2)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

4 a 1 (1) x,y,z [u,v,w] (2) x,y,z+1/2 [u,v,w]

Symmetry of Special Projections

Along [0,0,1] \text{c.P}1m1 \quad Along [1,0,0] \ P_{2a11} \quad Along [0,1,0] \ P_{2a1} 
\text{a}^* = -b \quad \text{b}^* = a_p \quad \text{a}^* = c/2 \quad \text{b}^* = a/2 + c/2

Origin at 0,0,z \quad \text{Origin at } x,0,0 \quad \text{Origin at } 0,y,0

9.4.48 - 1 - 73
P2/m
10.1.49

2/m
P12/m1

Monoclinic

Origin at center (2/m)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(2) 2 0,y,0
(3) 1 0,0,0
(4) m x,0,z

(1 |0,0,0)
(2 |0,0,0)
(3 |0,0,0)
(4 |0,0,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 n m</td>
<td>x,1/2,z [0,v,0]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 m m</td>
<td>x,0,z [0,v,0]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 l 2</td>
<td>1/2,y,1/2 [0,v,0]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 k 2</td>
<td>0,y,1/2 [0,v,0]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 j 2</td>
<td>1/2,y,0 [0,v,0]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 i 2</td>
<td>0,y,0 [0,v,0]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] p2'mm'  
Along [1,0,0] p2'mm'  
Along [0,1,0] p2111'

\[ a^* = -b \quad b^* = a \]

Origin at 0,0;z

Origin at x,0,0

Origin at 0,y,0
Origin at center (2/m1')

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

1. $1$ 
   $0,0,0$

2. $2,0,y,0$
   $0,0,0$

3. $1$$0,0,0$
   $0,0,0$

4. $m,x,0,z$
   $m,0,0,0$

For 1' + set

1'. $1'$
   $0,0,0$

2'. $2',0,y,0$
   $0,0,0$

3'. $1<0,0,0$
   $0,0,0$

4'. $m',x,0,z$
   $m',0,0,0$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Site Symmetry</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>+</td>
<td>1'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>2 n</td>
<td>m1'</td>
<td>(2) x,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 m</td>
<td>m1'</td>
<td>(3) x,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 l</td>
<td>21'</td>
<td>(4) x,y,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 k</td>
<td>21'</td>
<td>0,y,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 j</td>
<td>21'</td>
<td>1/2,y,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 i</td>
<td>21'</td>
<td>0,y,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 h</td>
<td>2/m1'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 g</td>
<td>2/m1'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 f</td>
<td>2/m1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 e</td>
<td>2/m1'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 d</td>
<td>2/m1'</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 c</td>
<td>2/m1'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 b</td>
<td>2/m1'</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a</td>
<td>2/m1'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm1'  \( a^* = a, \quad b^* = b \)
- Along [1,0,0] p2mm1'  \( a^* = b, \quad b^* = c, \quad a^* = c, \quad b^* = a \)

Origin at 0,0,z  \( \text{Origin at } x,0,0 \)  \( \text{Origin at } 0,y,0 \)
**Origin** at center (2/m)

**Asymmetric unit**
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\]

**Symmetry Operations**

1. \(1\)  \(1 \mid 0,0,0\)
2. \(2'\)  \(0,0,0\)
3. \(1'\)  \(0,0,0\)
4. \(m\)  \(x,0,z\)

\(2'/m\)  \(2'/m\)  Monoclinic

10.3.51  P12'/m1
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Positions</strong></td>
<td><strong>Coordinates</strong></td>
</tr>
<tr>
<td>o  1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>n m 2</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>m m 2</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>l 2'</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>k 2'</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>j 2'</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>i 2'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>h 2'm</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>g 2'm</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>f 2'/m</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>e 2'/m</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>d 2'/m</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>c 2'/m</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>b 2'/m</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>a 2'/m</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2nm
  - \( a^* = a \)
  - \( b^* = b \)
  - Origin at 0,0,z

- Along [1,0,0] p2mm
  - \( a^* = b \) \( b^* = c \)
  - Origin at x,0,0

- Along [0,1,0] p2111
  - \( a^* = c \) \( b^* = a \)
  - Origin at 0,y,0
Origin at center (2/m')

Asymmetric unit: $0 \leq x < 1/2; \ 0 \leq y < 1/2; \ 0 \leq z \leq 1$

Symmetry Operations:

1. $1$
   - $(1, 0, 0, 0)$
2. $2 \ y, 0, 0$
   - $(2, 0, 0, 0)$
3. $T' \ 0, 0, 0$
   - $(3, 0, 0, 0)'$
4. $m' \ x, 0, z$
   - $(4, 0, z, 0)'$
Continued

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 o 1</td>
<td>x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 n m'</td>
<td>x,1/2,z [u,0,w]</td>
<td>x,1/2,z [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 m m'</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 l 2</td>
<td>1/2,y,1/2 [0,v,0]</td>
<td>1/2,y,1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 k 2</td>
<td>0,y,1/2 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 j 2</td>
<td>1/2,y,0 [0,v,0]</td>
<td>1/2,y,0 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 i 2</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>1 h 2/m'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 g 2/m'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 f 2/m'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 e 2/m'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 d 2/m'</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 c 2/m'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 b 2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a 2/m'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2m'm'  
Along [1,0,0]  p2m'm'  
Along [0,1,0]  p211

a* = a  b* = b  
a* = b  b* = c  
a* = c  b* = a  

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center (2/m')

Asymmetric unit  
0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1

Symmetry Operations

(1) 1  
(1 | 0,0,0)  

(2) 2' 0, y, 0  
(2 | 0,0,0)'  

(3) 1 0, 0, 0  
(1 | 0,0,0)  

(4) m' x, 0, z  
(m | 0,0,0)'
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

| Mult. | Wyckoff | Coordinates          |  | Coordinates          |
|-------|---------|----------------------|  |----------------------|
| 4     | o 1     | (1) x,y,z [u,v,w]    | 2 | (2) x,y,z [u,v,w]    |
| 2     | n m'    | x,1/2,z [u,0,w]      | 2 | x,1/2,z [u,0,w]      |
| 2     | m m'    | x,0,z [u,0,w]        | 2 | x,0,z [u,0,w]        |
| 2     | l 2'    | 1/2,y,1/2 [u,0,w]    | 2 | 1/2,y,1/2 [u,0,w]    |
| 2     | k 2'    | 0,y,1/2 [u,0,w]      | 2 | 0,y,1/2 [u,0,w]      |
| 2     | j 2'    | 1/2,y,0 [u,0,w]      | 2 | 1/2,y,0 [u,0,w]      |
| 2     | i 2'    | 0,y,0 [u,0,w]        | 2 | 0,y,0 [u,0,w]        |
| 1     | h 2'/m' | 1/2,1/2,1/2 [u,0,w]  | 1 | 1/2,1/2,1/2 [u,0,w]  |
| 1     | g 2'/m' | 1/2,0,1/2 [u,0,w]    | 1 | 1/2,0,1/2 [u,0,w]    |
| 1     | f 2'/m' | 0,1/2,1/2 [u,0,w]    | 1 | 0,1/2,1/2 [u,0,w]    |
| 1     | e 2'/m' | 1/2,1/2,0 [u,0,w]    | 1 | 1/2,1/2,0 [u,0,w]    |
| 1     | d 2'/m' | 1/2,0,0 [u,0,w]      | 1 | 1/2,0,0 [u,0,w]      |
| 1     | c 2'/m' | 0,0,1/2 [u,0,w]      | 1 | 0,0,1/2 [u,0,w]      |
| 1     | b 2'/m' | 0,1/2,0 [u,0,w]      | 1 | 0,1/2,0 [u,0,w]      |
| 1     | a 2'/m' | 0,0,0 [u,0,w]        | 1 | 0,0,0 [u,0,w]        |

Symmetry of Special Projections

Along [0,0,1]  p2'm'  Along [1,0,0]  p2'm'  Along [0,1,0]  p2'11
\(a^* = a,\ b^* = b\)  \(a^* = -c,\ b^* = b\)  \(a^* = c,\ b^* = a\)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
P2a 2/m
10.6.54

2/m1′
P2a12/m1

Monoclinic

Origin at center (2/m)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,y,0
(2|0,0,0)

(3) 1 0,0,0
(1|0,0,0)

(4) m x,0,z
(m|0,0,0)

For (1,0,0)′ + set

(1) t′ (1,0,0)
(1|1,0,0)′

(2) 2′ 1/2,y,0
(2|1,0,0)′

(3) 1′ 1/2,0,0
(1|1,0,0)′

(4) a′ (1,0,0) x,0,z
(m|1,0,0)′
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Multiplicity</strong>, <strong>Wyckoff letter</strong>, <strong>Site Symmetry</strong></td>
<td></td>
</tr>
<tr>
<td>(0,0,0) + (1,0,0)' +</td>
<td></td>
</tr>
<tr>
<td>8 0 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 n m</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>4 m m</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 l 2'</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 k 2</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 j 2'</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 i 2</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>2 h 2'/m</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 g 2'/m</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 f 2/m</td>
<td>0,1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>2 e 2'/m</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d 2'/m</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 c 2/m</td>
<td>0,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>2 b 2/m</td>
<td>0,1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>2 a 2/m</td>
<td>0,0,0 [0,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_2a,2mm  
\[ a^* = a, \quad b^* = b \]
Origin at 1/2,0,z

Along [1,0,0]  p2mm1'  
\[ a^* = b, \quad b^* = c \]
Origin at x,0,0

Along [0,1,0]  p2111'  
\[ a^* = c, \quad b^* = a \]
Origin at 0,y,0
Origin at center (2/m)

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) \( \bar{1} \)  
(0,0,0)  

(2) \( 2 \)  
0,y,0  

(3) \( \bar{1} \)  
0,0,0  

(4) \( m \)  
x,0,z  

\( (m,0,0) \)

For (0,1,0)' + set

(1) \( t' \)  
(0,1,0)  

(2) \( 2' \)  
(0,1,0)'  

(3) \( \bar{1}' \)  
0,1/2,0  

(4) \( m' \)  
x,1/2,z  

\( (m',0,1,0)' \)
Generators selected  (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 n m'</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4 m m</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 l 2</td>
<td>1/2,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 k 2</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 j 2</td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 i 2</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>2 h 2/m'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 g 2/m</td>
<td>1/2,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>2 f 2/m'</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 e 2/m'</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d 2/m</td>
<td>1/2,0,0 0,v,0</td>
</tr>
<tr>
<td>2 c 2/m</td>
<td>0,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>2 b 2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 2/m</td>
<td>0,0,0 [0,v,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,1/2,z</th>
<th>Origin at x,1/2,0</th>
<th>Origin at 0,y,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = -b)</td>
<td>(b^* = a_p)</td>
<td>(a^* = c)</td>
</tr>
<tr>
<td>(b^* = a_p)</td>
<td>(a^* = b)</td>
<td>(b^* = a)</td>
</tr>
</tbody>
</table>
Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1 | 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(2) & \quad 2 \quad 0,y,0 \\
& \quad (0,0,0)
\end{align*}
\]

\[
\begin{align*}
(3) & \quad \overline{1} \quad 0,0,0 \\
& \quad (1 | 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(4) & \quad m \quad x,0,z \\
& \quad (0,0,0)
\end{align*}
\]

For \((1,0,0) + \) set

\[
\begin{align*}
(1) & \quad t' \quad (1,0,0) \\
& \quad (1 | 1,0,0)
\end{align*}
\]

\[
\begin{align*}
(2) & \quad 2' \quad 1/2,y,0 \\
& \quad (0,0,0)
\end{align*}
\]

\[
\begin{align*}
(3) & \quad \overline{1}' \quad 1/2,0,0 \\
& \quad (1 | 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(4) & \quad a' \quad (1,0,0) \quad x,0,z \\
& \quad (0,0,0)
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity,  Coordinates
Wyckoff letter,  (0,0,0) + (1,0,0)' +
Site Symmetry.

(0,0,0) + (1,0,0)'
(0,0,0) + (1,0,0)

8  o  1  (1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) x,y,z [u,v,w]  (4) x,y,z [u,v,w]
4  n  m'  x,1/2,z [u,0,w]  x,1/2,z [u,0,w]
4  m  m  x,0,z [0,v,0]  x,0,z [0,v,0]
4  l  2'  1/2,y,1/2 [u,0,w]  1/2,y,1/2 [u,0,w]
4  k  2  0,y,1/2 [0,v,0]  0,y,1/2 [0,v,0]
4  j  2'  1/2,y,0 [u,0,w]  1/2,y,0 [u,0,w]
4  i  2  0,y,0 [0,v,0]  0,y,0 [0,v,0]
2  h  2'/m'  1/2,1/2,1/2 [u,0,w]
2  g  2'/m  1/2,0,1/2 [0,0,0]
2  f  2/m'  0,1/2,1/2 [0,0,0]
2  e  2'/m'  1/2,1/2,0 [u,0,w]
2  d  2'/m  1/2,0,0 [0,0,0]
2  c  2/m  0,0,1/2 [0,v,0]
2  b  2'/m'  0,1/2,0 [0,0,0]
2  a  2/m  0,0,0 [0,v,0]

Symmetry of Special Projections

Along [0,0,1]  p_2mm  Along [1,0,0]  p_2mm1'  Along [0,1,0]  p2_11  
\[a^* = a, \quad b^* = b\]  \[a^* = b, \quad b^* = c, \quad a = c, \quad b^* = a\]
Origin at 1/2,0,z  Origin at x,0,0  Origin at 0,y,0
\[ P_{2b}\ 2'/m \]

Origin at center (2'/m)

Asymmetric unit \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0)\) + set

\[(1) \ 1 \quad (2) \ 2' \quad (3) \ \bar{1}' \quad (4) \ m \]
\[(1 \ 0,0,0) \quad (2 \ y,0,0) \quad (3 \ |0,0,0) \bar{1}' \quad (m \ x,0,z) \]

For \((0,1,0)'\) + set

\[(1) \ t' \quad (2) \ 2 \quad (3) \ \bar{1} \quad (4) \ m' \]
\[(1 \ 0,1,0) \quad (2 \ y,0,0) \quad (3 \ |0,0,0) \bar{1} \quad (m' \ x,1/2,z) \]

\[ 2/m1' \]

\[ P_{2b12'/m1} \]

Monoclinic
Generators selected (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(0,1,0) ' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 n m'</td>
<td>x,1/2,z [u,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 m m</td>
<td>x,0,z [0,v,0]</td>
<td>x,1/2,z [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 l 2'</td>
<td>1/2,y,1/2 [u,0,w]</td>
<td>1/2,y,1/2 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 k 2'</td>
<td>0,y,1/2 [u,0,w]</td>
<td>0,y,1/2 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 j 2'</td>
<td>1/2,y,0 [u,0,w]</td>
<td>1/2,y,0 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 i 2'</td>
<td>0,y,0 [u,0,w]</td>
<td>0,y,0 [u,0,w]</td>
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</tr>
<tr>
<td>2 h 2'/m'</td>
<td>1/2,1/2,1/2 [u,0,w]</td>
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<tr>
<td>2 g 2'/m</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 f 2'/m'</td>
<td>0,1/2,1/2 [u,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 e 2'/m'</td>
<td>1/2,1/2,0 [u,0,w]</td>
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<td></td>
</tr>
<tr>
<td>2 d 2'/m</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 2'/m</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b 2'/m'</td>
<td>0,1/2,0 [u,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a 2'/m</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a}.2mm   Along [1,0,0] p_{2a}.2mm   Along [0,1,0] p_{2111}'
\( \mathbf{a}^\ast = -\mathbf{b} \quad \mathbf{b}^\ast = \mathbf{a} \_p \)
\( \mathbf{a}^\ast = \mathbf{b} \quad \mathbf{b}^\ast = \mathbf{c} \_p \)
\( \mathbf{a}^\ast = \mathbf{c} \quad \mathbf{b}^\ast = \mathbf{a} \)
Origin at 0,1/2,z
Origin at x,1/2,0
Origin at 0,y,0
**Symmetry Operations**

For \( (0,0,0) \) + set

1. \( \bar{1} \) \( (1|0,0,0) \)
2. \( 2 \) \( 0,y,0 \)
3. \( \bar{1} \) \( 0,0,0 \)
4. \( m' \) \( x,0,z \)

For \( (0,0,1)' \) + set

1. \( \bar{1} \) \( (0,0,1) \)
2. \( 2' \) \( 0,y,1/2 \)
3. \( \bar{1} \) \( 0,0,1/2 \)
4. \( c \) \( (0,0,1) \)

**Origin** at center (\( 2/m' \))

**Asymmetric unit**

\( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)’ +</td>
</tr>
<tr>
<td>4 n m’</td>
<td>x,1/2,z [u,0,w]</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4 m’</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
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<tr>
<td>4 l 2’</td>
<td>1/2,y,1/2 [u,0,w]</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 k 2’</td>
<td>0,y,1/2 [u,0,w]</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 j 2</td>
<td>1/2,y,0 [0,v,0]</td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 i 2</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>2 h 2’/m’</td>
<td>1/2,1/2,1/2 [u,0,w]</td>
<td>2 g 2’/m’ 1/2,0,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 f 2’/m’</td>
<td>0,1/2,1/2 [u,0,w]</td>
<td>2 e 2/m’ 1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d 2/m’</td>
<td>1/2,0,0 [0,0,0]</td>
<td>2 c 2’/m’ 0,0,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 b 2/m’</td>
<td>0,1/2,0 [0,0,0]</td>
<td>2 a 2/m’ 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm1’  
  \[ a^* = a_b \quad b^* = b \]  
  Origin at 0,0,z

- Along [1,0,0] p2a-2m’m’  
  \[ a^* = -c_b \quad b^* = b \]  
  Origin at 0,y,0

- Along [0,1,0] p2a-211  
  \[ a^* = c \quad b^* = a \]  
  Origin at x,0,0
Origin at 1 on 2₁

Asymmetric unit

\[ 0 < x < 1; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1 \]

Symmetry Operations

(1) 1
(2) \( \bar{2} \quad (0,1/2,0) \quad 0,y,0 \)
(3) \( \bar{1} \quad 0,0,0 \)
(4) \( m \quad x,1/4,z \)
(1) \( (0,0,0) \)
(2) \( (2_y,0,1/2,0) \)
(3) \( (1,0,0,0) \)
(4) \( (m,0,1/2,0) \)
Generators selected  (1); (1,0,0); (0,1,0); (0,0,1); (2); (3).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

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<tr>
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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>2 e m</td>
<td>x,1/4,z [0,v,0]</td>
<td>x,3/4,z [0,v,0]</td>
</tr>
<tr>
<td>2 d 1</td>
<td>1/2,0,1/2 [u,v,w]</td>
<td>1/2,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 c 1</td>
<td>0,0,1/2 [u,v,w]</td>
<td>0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 b 1</td>
<td>1/2,0,0 [u,v,w]</td>
<td>1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>2 a 1</td>
<td>0,0,0 [u,v,w]</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  p2'mg'  
\( a^* = -b \quad b^* = a_p \)

Origin at 0,0,z  

Along [1,0,0]  p2'mg'  
\( a^* = b \quad b^* = c_p \)

Origin at x,0,0  

Along [0,1,0]  p2111'  
\( a^* = c \quad b^* = a \)

Origin at 0,y,0
Origin at $1'$ on $2_1$'

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq 1/4$; $0 \leq z \leq 1$

Symmetry Operations

For 1 + set

1. $1$  
   $(1 \mid 0,0,0)$

2. $2$  
   $(2 \mid 0,1/2,0)$, $0,y,0$
   $(2_g \mid 0,1/2,0)$

3. $m$  
   $(3 \mid 0,0,0)$
   $(m \mid 0,1/2,0)$

For 1' + set

1. $1'$  
   $(1 \mid 0,0,0)'$

2. $2'$  
   $(2 \mid 0,1/2,0)$, $0,y,0$
   $(2_g \mid 0,1/2,0)'$

3. $m'$  
   $(3 \mid 0,0,0)'$
   $(m \mid 0,1/2,0)'$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>1 +</td>
</tr>
<tr>
<td>4 f 11' (1) x,y,z [0,0,0]</td>
<td>(2) x,y+1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 e m1' x,1/4,z [0,0,0]</td>
<td>x,3/4,z [0,0,0]</td>
</tr>
<tr>
<td>2 d 1' 1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 1' 0,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 1' 1/2,0,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 1' 0,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p2mg1'  
Along [1,0,0] p2mg1'  
Along [0,1,0] p2111'  
\(a^* = -b\) \(b^* = a_p\)  
\(a^* = b\) \(b^* = c_p\)  
\(a^* = c\) \(b^* = a\)  
Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at 1 on 2

Asymmetric unit
0 ≤ x ≤ 1; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2' (0,1/2,0) 0,y,0
(2_2 | 0,1/2,0)

(3) 1' 0,0,0
(1 | 0,0,0)

(4) m x,1/4,z
(m_2 | 0,1/2,0)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>4 f 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>2 e m x,1/4,z [0,v,0]</td>
<td>x,3/4,z [0,v,0]</td>
</tr>
<tr>
<td>2 d 1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 0,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 1/2,0,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 0,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mg  
  \( \mathbf{a}^* = -\mathbf{b} \quad \mathbf{b}^* = \mathbf{a} \)  
  Origin at 0,0,z

- Along [1,0,0] p2mg  
  \( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)  
  Origin at x,0,0

- Along [0,1,0] p2111'  
  \( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a} \)  
  Origin at 0,y,0
**Origin** at \( \overline{1} \) on 2₁

**Asymmetric unit**  
\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

1. \( 1 \)  
   \( (1 \mid 0,0,0) \)

2. \( 2 \)  
   \( (2_y \mid 0,1/2,0) \)

3. \( \overline{1} \)  
   \( (1 \mid 0,0,0)' \)

4. \( m' \)  
   \( (m_y \mid 0,1/2,0)' \)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>f</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y + 1/2, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(3) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(4) x, y + 1/2, z [u, v, w]</td>
</tr>
<tr>
<td>e</td>
<td>m'</td>
</tr>
<tr>
<td></td>
<td>x, 1/4, z [u, 0, w]</td>
</tr>
<tr>
<td>d</td>
<td>t'</td>
</tr>
<tr>
<td></td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>c</td>
<td>t'</td>
</tr>
<tr>
<td></td>
<td>0, 0, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>b</td>
<td>t'</td>
</tr>
<tr>
<td></td>
<td>1/2, 0, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>a</td>
<td>t'</td>
</tr>
<tr>
<td></td>
<td>0, 0, 0 [0, 0, 0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0, 0, 1] p2m'g'   Along [1, 0, 0] p2m'g'   Along [0, 1, 0] p211'  
\[a^* = -b, \quad b^* = a_p \] \[a^* = b, \quad b^* = c_p \] \[a^* = c, \quad b^* = a \]  
Origin at 0, 0, z        Origin at x, 0, 0        Origin at 0, y, 0
Origin at 1 on 2pr

Asymmetric unit

0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2pr (0,1/2,0) 0,y,0
(2y | 0,1/2,0)’

(3) 1 0,0,0
(1 | 0,0,0)

(4) m’ x,1/4,z
(my | 0,1/2,0)’

P21,’/m’

11.5.63

P12, ’/m’1

Monoclinic
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>4 f 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y+1/2,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>2 e m'</td>
<td>x,1/4,z [u,0,w] x,3/4,z [u,0,w]</td>
</tr>
<tr>
<td>2 d</td>
<td>1/2,0,1/2 [u,v,w] 1/2,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 c</td>
<td>0,0,1/2 [u,v,w] 0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 b</td>
<td>1/2,0,0 [u,v,w] 1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>2 a</td>
<td>0,0,0 [u,v,w] 0,1/2,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'm'g  
Along [1,0,0] p2'm'g  
Along [0,1,0] p2'11

\[ a^* = -b \quad b^* = a \]

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at \( \bar{1} \) on \( 2_1 \)

Asymmetric unit:
\[ 0 < x < 1; \quad 0 < y < 1/4; \quad 0 < z < 1 \]

Symmetry Operations

For \((0,0,0)\) + set:

(1) \( \bar{1} \)
(1) \((0,0,0)\)

(2) \( 2(0,1/2,0) \)
(2) \((0,1/2,0)\)

(3) \( \bar{1}(0,0,0) \)
(3) \((0,0,0)\)

(4) \( m \)
(4) \((x,1/4,z)\)
\((m_y,0,1/2,0)\)

For \((1,0,0)\)' + set:

(1) \( t' \)
(1) \((1,0,0)\)'

(2) \( 2'(0,1/2,0) \)
(2) \((0,1/2,0)\)'

(3) \( \bar{1}' \)
(3) \((1/2,0,0)\)'

(4) \( a' \)
(4) \((x,1/4,z)\)
\((m_y,1,1/2,0)\)'
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m</td>
<td>x,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>0,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2b.2mg</th>
<th>Along [1,0,0]</th>
<th>p2mg1'</th>
<th>Along [0,1,0]</th>
<th>p2111'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a_p</td>
<td>a* = b</td>
<td>b* = c_p</td>
<td>a* = c</td>
<td>b* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin at \( \overline{1} \) on \( 2_1 \)

Asymmetric unit

\( 0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \( (0,0,0) + \) set

1. \( 1 \)
   \( (1|0,0,0) \)

2. \( 1 \)
   \( (0,1/2,0) \)
   \( (2|0,1/2,0) \)

3. \( \bar{1} \)
   \( (0,0,0) \)
   \( (0,0,0)' \)

4. \( m' \)
   \( x,1/4,z \)
   \( (0,1/2,0)' \)

For \( (0,0,1)' + \) set

1. \( t' \)
   \( (0,0,1) \)
   \( (1|0,0,1)' \)

2. \( 2' \)
   \( (0,1/2,0) \)
   \( (2|0,1/2,1)' \)

3. \( \bar{1} \)
   \( (0,0,1/2) \)
   \( (0,0,1) \)

4. \( c \)
   \( (0,0,1) \)
   \( x,1/4,z \)
   \( (0,1/2,1) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(0,0,0) + (0,0,1) +</td>
</tr>
<tr>
<td>4 e m'</td>
<td></td>
</tr>
<tr>
<td>4 d ( \bar{1} )</td>
<td></td>
</tr>
<tr>
<td>4 c ( \bar{1} )</td>
<td></td>
</tr>
<tr>
<td>4 b ( \bar{1} )</td>
<td></td>
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<tr>
<td>4 a ( \bar{1} )</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg1' 
Along [1,0,0] p2inv2m'g' 
Along [0,1,0] p2a*211 
\( a^* = -b \) \( b^* = a_p \) 
\( a^* = b \) \( b^* = c_p \) 
\( a^* = c \) \( b^* = a \) 
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at center \((2/m)\)

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) \ 1 & \quad (2) \ 2 \ 0,y,0 & \quad (3) \ \bar{1} \ 0,0,0 \\
(1,0,0,0) & \quad (2,0,0,0) & \quad (1,0,0,0) \\
(4) \ m \ x,0,z & \quad (m,0,0,0)
\end{align*}
\]

For \((1/2,1/2,0) + \) set

\[
\begin{align*}
(1) \ t & \quad (2) \ 2 \ (0,1/2,0) \ 1/4,y,0 & \quad (3) \ \bar{1} \ 1/4,1/4,0 \\
(1,1/2,1/2,0) & \quad (2,1/2,1/2,0) & \quad (1,1/2,1/2,0) \\
(4) \ a \ (1/2,0,0) \ x,1/4,z & \quad (m,1/2,1/2,0)
\end{align*}
\]
Continued 12.1.66 C2/m

Generators selected  (1); t(1,0,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>4 i m</td>
<td>x,0,z [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 h 2</td>
<td>0,y,1/2 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 g 2</td>
<td>0,y,0 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 f 1</td>
<td>1/4,1/4,1/2 [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 e 1</td>
<td>1/4,1/4,0 [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 d 2/m</td>
<td>0,1/2,1/2 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 2/m</td>
<td>0,0,1/2 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b 2/m</td>
<td>0,1/2,0 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a 2/m</td>
<td>0,0,0 [0,v,0]</td>
<td></td>
<td></td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2' mm'</th>
<th>Along [1,0,0]</th>
<th>p2' mm'</th>
<th>Along [0,1,0]</th>
<th>p2111'</th>
</tr>
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<tr>
<td>a' = -b</td>
<td>b' = a_p</td>
<td>a' = b/2</td>
<td>b' = c_p</td>
<td>a' = c</td>
<td>b' = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
C2/m1' 2/m1' Monoclinic

12.2.67 C12/m11'

Origin at center (2/m1')

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0) (2) 2' 0,y,0 (2'|0,0,0) (3) 1' 0,0,0 (1'|0,0,0) (4) m x,0,z (m|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1|1/2,1/2,0) (2) 2 (0,1/2,0) 1/4,y,0 (2'|1/2,1/2,0) (3) 1 1/4,1/4,0 (1|1/2,1/2,0) (4) a (1/2,0,0) x,1/4,z (m|1/2,1/2,0)

For (0,0,0)' + set

(1) 1' (1|0,0,0)' (2) 2' 0,y,0 (2'|0,0,0)' (3) 1' 0,0,0 (1'|0,0,0)' (4) m' x,0,z (m|0,0,0)'

For (1/2,1/2,0) + set

(1) t' (1/2,1/2,0) (1|1/2,1/2,0) (2) 2' (0,1/2,0) 1/4,y,0 (2'|1/2,1/2,0) (3) 1' 1/4,1/4,0 (1|1/2,1/2,0) (4) a' (1/2,0,0) x,1/4,z (m|1/2,1/2,0)'

12.2.67 - 1 - 110
### Generators selected

(1); t(1,0,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

### Positions

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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8  j  11'  (1) x,y,z [0,0,0]</td>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>4  i  m1'  x,0,z [0,0,0]</td>
<td>x,0,z [0,0,0]</td>
</tr>
<tr>
<td>4  h  21'  0,y,1/2 [0,0,0]</td>
<td>0,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4  g  21'  0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4  f  11'  1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4  e  11'  1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2  d  2/m1'  0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2  c  2/m1'  0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2  b  2/m1'  0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2  a  2/m1'  0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] c2mm1'  
  a* = a  b* = b

- Along [1,0,0] p2mm1'  
  a* = b/2  b* = c

- Along [0,1,0] p2111'  
  a* = c  b* = a/2

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
C2'/m  2'/m  Monoclinic

12.3.68  C12'/m1

Origin  at center (2'/m)

Asymmetric unit  
0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/4;  0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1  (2) 2'  0,y,0  (3) 1  (4) m  x,0,z
   (1|0,0,0)   (2'|0,0,0)   (1|0,0,0)'   (m|0,0,0)

For (1/2,1/2,0) + set

(1) t  (2) 2'  (0,1/2,0)  1/4,y,0  (3) 1'  1/4,1/4,0  (4) a  (1/2,0,0)  x,1/4,z
   (1|1/2,1/2,0)   (2'|1/2,1/2,0)   (1'|1/2,1/2,0)'   (m|1/2,1/2,0)

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x̄,y,z [ū,v̄,w]</td>
<td>(3) x̄,y,z [ū,v̄,w]</td>
</tr>
<tr>
<td>4 i m</td>
<td>x,0,z [0,v,0]</td>
<td>x̄,0,z [0̄,v̄,0]</td>
<td></td>
</tr>
<tr>
<td>4 h 2'</td>
<td>0,y,1/2 [u,0,w]</td>
<td>0̄,y,1/2 [ū,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 g 2'</td>
<td>0,y,0 [u,0,w]</td>
<td>0̄,y,0 [ū,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 f 1̊</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e 1̊</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 d 2'/m</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 2'/m</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b 2'/m</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a 2'/m</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm  Along [1,0,0] p2mm  Along [0,1,0] p2111'

\( \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \)  \( \mathbf{a}^* = \mathbf{b}/2, \mathbf{b}^* = \mathbf{c}, \mathbf{c}^* = \mathbf{a}/2 \)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
C2/m' 2/m' Monoclinic

12.4.69 12.4.69 C12/m'1

**Origin** at center (2/m')

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

**Symmetry Operations**

For (0,0,0) + set

(1) 1
(2) 2 0,y,0
(3) 1' 0,0,0
(4) m' x,0,z

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(2) 2 (0,1/2,0) 1/4,y,0
(3) 1' 1/4,1/4,0
(4) a' (1/2,0,0) x,1/4,z

(1) 1 (0,0,0)
(2) 2 (0,0,0)
(3) 1' (0,0,0)'
(4) m' (0,0,0)'

(1) t (1/2,1/2,0)
(2) 2 (1/2,0,0)
(3) 1' (1/2,1/2,0)'
(4) a' (1/2,1/2,0) x,1/4,z

(m, 1/2, 0, 0)'

(m, 1/2, 1/2, 0)'
Generators selected  
(1); t(1,0,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Position

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 i m'</td>
<td>x,0,z [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 h 2</td>
<td>0,y,1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 g 2</td>
<td>0,y,0 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 f 1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>4 e 1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 d 0,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b 0,1/2,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a 0,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2m' a* = a, b* = b
- Along [1,0,0] p2m' a* = b/2, b* = c
- Along [0,1,0] p211 a* = c, b* = a/2

Origin at 0,0,z
Origin at x,0,0
Origin at 0,y,0
**C2′/m′ 2′/m′ Monoclinic**

12.5.70  
C12′/m′1

**Origin** at center (2′/m′)

**Asymmetric unit**  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

**Symmetry Operations**

For (0,0,0) + set

(1) \(1\)  
\(0,0,0\)

(2) \(2′\) \(y,0,0\)
\(0,0,0′\)

(3) \(\bar{1}\) \(0,0,0\)

(4) \(m′\) \(x,0,z\)
\(m′,0,0′\)

For (1/2,1/2,0) + set

(1) \(t\) \(1/2,1/2,0\)
\(1/2,1/2,0\)

(2) \(2′\) \(0,1/2,0\)
\(1/4,y,0\)

(3) \(\bar{1}\) \(1/4,1/4,0\)

(4) \(a′\) \(1/2,0,0\)
\(x,1/4,z\)
\(m′,1/2,1/2,0′\)

\(1/2,1/2,0′\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**
Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1</td>
<td>(1) x,y,z ([u,v,w])</td>
</tr>
<tr>
<td>4 i m'</td>
<td>x,0,z ([u,0,w])</td>
</tr>
<tr>
<td>4 h 2'</td>
<td>0,y,1/2 ([u,0,w])</td>
</tr>
<tr>
<td>4 g 2'</td>
<td>0,y,0 ([u,0,w])</td>
</tr>
<tr>
<td>4 f 1</td>
<td>1/4,1/4,1/2 ([u,v,w])</td>
</tr>
<tr>
<td>4 e 1</td>
<td>1/4,1/4,0 ([u,v,w])</td>
</tr>
<tr>
<td>2 d 2'/m'</td>
<td>0,1/2,1/2 ([u,0,w])</td>
</tr>
<tr>
<td>2 c 2'/m'</td>
<td>0,0,1/2 ([u,0,w])</td>
</tr>
<tr>
<td>2 b 2'/m'</td>
<td>0,1/2,0 ([u,0,w])</td>
</tr>
<tr>
<td>2 a 2'/m'</td>
<td>0,0,0 ([u,0,w])</td>
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</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>c2'm'</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2'm'</td>
</tr>
<tr>
<td>Along [0,1,0]</td>
<td>p2'11</td>
</tr>
</tbody>
</table>

\[ \mathbf{a}^* = \mathbf{a}_\perp, \quad \mathbf{b}^* = \mathbf{b} \]

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
C\textsubscript{2c}2/m  
12.6.71  
C\textsubscript{2c}12/m1  

Monoclinic

Origin at center (2/m)

Asymmetric unit
0 \leq x \leq 1/2; 0 \leq y \leq 1/4; 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) \text{1}  
(1 | 0,0,0)

(2) \text{2}  y,0,0  
(2 | 0,0,0)

(3) \text{1}  0,0,0  
(1 | 0,0,0)

(4) \text{m}  x,0,z  
(m | 0,0,0)

For (1/2,1/2,0) + set

(1) \text{t}  (1/2,1/2,0)  
(1 | 1/2,1/2,0)

(2) \text{2}  (0,1/2,0)  1/4,y,0  
(2 | 1/2,1/2,0)

(3) \text{1}  1/4,1/4,0  
(1 | 1/2,1/2,0)

(4) \text{a}  (1/2,0,0)  x,1/4,z  
(m | 1/2,1/2,0)

For (0,0,1) + set

(1) \text{t}  (0,0,1)  
(1 | 0,0,1)

(2) \text{2}  y,1/2  
(2 | 0,0,1)

(3) \text{1}  0,0,1/2  
(1 | 0,0,1)

(4) \text{c}  (0,0,1)  x,0,z  
(m | 0,0,1)

For (1/2,1/2,1) + set

(1) \text{t}  (1/2,1/2,1)  
(1 | 1/2,1/2,1)

(2) \text{2}  (0,1/2,0)  1/4,y,1/2  
(2 | 1/2,1/2,1)

(3) \text{1}  1/4,1/4,1/2  
(1 | 1/2,1/2,1)

(4) \text{n}  (1/2,0,1)  x,1/4,z  
(m | 1/2,1/2,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

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<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>16 j</td>
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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v]</td>
</tr>
<tr>
<td>8 i m</td>
<td>0,0,z [0,v,0]</td>
<td>(3) x,y,z [u,v,w]</td>
<td>(4) x,y,z [u,v]</td>
</tr>
<tr>
<td>8 h 2'</td>
<td>0,y,1/2 [u,0,w]</td>
<td>0,y,1/2 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 g 2</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 f 1'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 e 1</td>
<td>1/4,1/4,0 [u,v,0]</td>
<td>3/4,1/4,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 d 2/m</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 c 2/m</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 b 2/m</td>
<td>0,1/2,0 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 a 2/m</td>
<td>0,0,0 [0,v,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2mm1'  
  \( a^* = a \quad b^* = b \)
- Along [1,0,0] p2111'  
  \( a^* = b/2 \quad b^* = c \)
- Along [0,1,0]  
  \( a^* = c \quad b^* = a/2 \)

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center (2/m)

Asymmetric unit \(0 \leq x \leq 1/2;\) \(0 \leq y \leq 1/4;\) \(0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \) set

1. \((1) 1 \) \((0,0,0)\)
   \((1) 0,0,0\)

2. \((2) 2 \) \(0,y,0\)
   \((2,0,0,0)\)

3. \((3) \bar{1} \) \(0,0,0\)
   \((1,0,0,0)\)

4. \((4) m \) \(x,0,z\)
   \((m,0,0,0)\)

For \((1/2,1/2,0) + \) set

1. \((1) t' \) \((1/2,1/2,0)\)
   \((1,1/2,1,2,0)\)

2. \((2) 2' \) \((0,1/2,0)\) \(1/4,y,0\)
   \((2,1/4,1/2,0)\)

3. \((3) \bar{1}' \) \(1/4,1/4,0\)
   \((1,1/2,1/2,0)\)

4. \((4) a' \) \((1/2,0,0)\) \(x,1/4,z\)
   \((m,0,0,0)\)

\[
\text{CP2/m} \quad \text{2/m1'} \quad \text{Monoclinic}
\]

\[
12.7.72 \quad \text{C} \quad 12/m1
\]
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,0)’ +</td>
</tr>
<tr>
<td>4 i m</td>
<td>x,0,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 h 2</td>
<td>0,y,1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 g 2</td>
<td>0,y,0 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 f 1/1</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e 1/1</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 d 2/m</td>
<td>0,1/2,1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 c 2/m</td>
<td>0,0,1/2 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 b 2/m</td>
<td>0,1/2,0 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2/m</td>
<td>0,0,0 [0,v,0]</td>
<td></td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \[c_p \cdot 2 \cdot \text{mm}^1\]  \[a^* = -b, \quad b^* = a_p\]  Origin at 0,0,z
Along [1,0,0] \[p2 \cdot \text{mm}^1\]  \[a^* = b/2, \quad b^* = c_p\]  Origin at x,0,0
Along [0,1,0] \[p2111^*\]  \[a^* = c, \quad b^* = a/2\]  Origin at 0,y,0
**Origin** at center \((2/m')\)

**Asymmetric unit** \(0 \leq x \leq 1/2;\) \(0 \leq y \leq 1/4;\) \(0 \leq z \leq 1\)

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 0, y, 0 \\
(3) & \quad 0, 0, 0 \\
(4) & \quad m', x, 0, z
\end{align*}
\]

For \((1/2,1/2,0) + \text{ set}\)

\[
\begin{align*}
(1) & \quad t \\
(2) & \quad 0, 1/2, 0 \\
(3) & \quad 1/4, 1/4, 0 \\
(4) & \quad a'(1/2, 0, 0)
\end{align*}
\]

For \((0,0,1)' + \text{ set}\)

\[
\begin{align*}
(1) & \quad t' \\
(2) & \quad 0, 0, 1/2 \\
(3) & \quad 0, 0, 1 \\
(4) & \quad c(0, 0, 1)
\end{align*}
\]

For \((1/2,1/2,1)' + \text{ set}\)

\[
\begin{align*}
(1) & \quad t' \\
(2) & \quad 0, 1/2, 0 \\
(3) & \quad 1/4, 1/4, 1/2 \\
(4) & \quad n(1/2, 0, 1)
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<td>(1/2,1/2,0) +</td>
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<tr>
<td>(0,0,1) +</td>
<td>(1/2,1/2,1) +</td>
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</table>

<table>
<thead>
<tr>
<th>Generators</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2mm1'  
\(a^* = a\) \(b^* = b\)  
Origin at 0,0,z

Along [1,0,0]  p22z2m'm'  
\(a^* = -c\) \(b^* = b/2\)  
Origin at x,0,0

Along [0,1,0]  p2z2.211  
\(a^* = c\) \(b^* = a/2\)  
Origin at 0,y,0
Origin at center (2'/m)

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

1. 1
   (1 | 0,0,0)
   (2) 2' 0,y,0
   (3) 1' 0,0,0
   (4) m  x,0,z

   (1 | 0,0,0)'
   (2 y | 0,0,0)'
   (1 & 0,0,0)'
   (m y | 0,0,0)

For (1/2,1/2,0)' + set

1. t' (1/2,1/2,0)
   (1 | 1/2,1/2,0)'

2. 2 (0,1/2,0) 1/4,y,0
   (2 | 1/2,1/2,0)

3. 1' 1/4,1/4,0
   (1 | 1/2,1/2,0)'

4. a' (1/2,0,0) x,1/4,z
   (m | 1/2,1/2,0)'

C_p2'/m 2m1' Monoclinic
12.9.74 C_p12'/m1
Generators selected  \((1); t(1,0,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1</td>
<td>(x,y,z)</td>
<td>([u,v,w])</td>
</tr>
<tr>
<td>4 i m</td>
<td>(x,0,z)</td>
<td>([0,v,0])</td>
</tr>
<tr>
<td>4 h 2'</td>
<td>0,y,1/2</td>
<td>([u,0,w])</td>
</tr>
<tr>
<td>4 g 2'</td>
<td>0,y,0</td>
<td>([u,0,w])</td>
</tr>
<tr>
<td>4 f 1</td>
<td>1/4,1/4,1/2</td>
<td>([u,v,w])</td>
</tr>
<tr>
<td>4 e 1</td>
<td>1/4,1/4,0</td>
<td>([u,v,w])</td>
</tr>
<tr>
<td>2 d 2'/m</td>
<td>0,1/2,1/2</td>
<td>([0,0,0])</td>
</tr>
<tr>
<td>2 c 2'/m</td>
<td>0,0,1/2</td>
<td>([0,0,0])</td>
</tr>
<tr>
<td>2 b 2'/m</td>
<td>0,1/2,0</td>
<td>([0,0,0])</td>
</tr>
<tr>
<td>2 a 2'/m</td>
<td>0,0,0</td>
<td>([0,0,0])</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: \(c_{\parallel}2\text{mm}\)
- **Along [1,0,0]**: \(p_{22}\cdot2\text{mm}\)
- **Along [0,1,0]**: \(p2111'\)

\(a^* = a\), \(b^* = b\)  
\(a^* = b/2\), \(b^* = c\)  
\(a^* = c\), \(b^* = a/2\)
C\textsubscript{p}2/m'

12.10.75

2/m1'

Monoclinic

C\textsubscript{p}12/m1'

**Origin** at center (2/m')

**Asymmetric unit**

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1 \]

**Symmetry Operations**

For (0,0,0) + set

(1) \textbf{1} \hspace{1cm} (2) \textbf{2} \hspace{1cm} (3) \textbf{1}' \hspace{1cm} (4) \textbf{m}'

\begin{align*}
(1) \text{ (0,0,0)} \hspace{1cm} (2) \text{ (0,y,0)} \hspace{1cm} (3) \text{ (0,0,0)'} \hspace{1cm} (4) \text{ (x,0,z)}
\end{align*}

(1) \text{ (1/2,1/2,0)} \hspace{1cm} (2) \text{ (0,1/2,0)} \hspace{1cm} (3) \text{ (1/4,1/4,0)} \hspace{1cm} (4) \text{ (1/2,0,0)}

\begin{align*}
(1) \text{ (1/2,1/2,0)'} \hspace{1cm} (2) \text{ (1/2,1/2,0)'} \hspace{1cm} (3) \text{ (1/2,1/2,0)'} \hspace{1cm} (4) \text{ (1/2,1/2,0)'}
\end{align*}

For (1/2,1/2,0) + set

\begin{align*}
(1) \text{ (1/2,1/2,0)} \hspace{1cm} (2) \text{ (0,1/2,0)} \hspace{1cm} (3) \text{ (1/4,1/4,0)} \hspace{1cm} (4) \text{ (1/2,0,0)}
\end{align*}

(1) \text{ (1/2,1/2,0)'} \hspace{1cm} (2) \text{ (1/2,1/2,0)'} \hspace{1cm} (3) \text{ (1/2,1/2,0)'} \hspace{1cm} (4) \text{ (1/2,1/2,0)'}
Generators selected  
(1); t(1,0,0); t(0,0,1); t(2,1,0); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,0)'</td>
<td>(1/2,1/2,0)'</td>
</tr>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,0)'</td>
<td>(1/2,1/2,0)'</td>
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<tr>
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<td>(1/2,1/2,0)'</td>
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<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,0)'</td>
<td>(1/2,1/2,0)'</td>
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</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c&lt;sub&gt;p&lt;/sub&gt;2m'm'</th>
<th>Along [1,0,0]</th>
<th>p&lt;sub&gt;2a&lt;/sub&gt;2m'm'</th>
<th>Along [0,1,0]</th>
<th>p&lt;sub&gt;2a&lt;/sub&gt;211</th>
</tr>
</thead>
<tbody>
<tr>
<td>a&lt;sup&gt;<em>&lt;/sup&gt; = a, b&lt;sup&gt;</em>&lt;/sup&gt; = b</td>
<td>a&lt;sup&gt;<em>&lt;/sup&gt; = b/2, b&lt;sup&gt;</em>&lt;/sup&gt; = c</td>
<td>a&lt;sup&gt;<em>&lt;/sup&gt; = -a/2, b&lt;sup&gt;</em>&lt;/sup&gt; = c</td>
<td>a&lt;sup&gt;<em>&lt;/sup&gt; = a, b&lt;sup&gt;</em>&lt;/sup&gt; = b</td>
<td>a&lt;sup&gt;<em>&lt;/sup&gt; = -a/2, b&lt;sup&gt;</em>&lt;/sup&gt; = c</td>
<td>a&lt;sup&gt;<em>&lt;/sup&gt; = a, b&lt;sup&gt;</em>&lt;/sup&gt; = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>
Origin at center (2'/m')

Asymmetric unit: $0 \leq x < 1/2$; $0 \leq y < 1/4$; $0 \leq z \leq 1$

Symmetry Operations:

For (0,0,0) + set:

1. $1$
   
   (1) $1$
   
   (2) $2'$, 0,y,0
   
   (3) 1, 0,0,0
   
   (4) $m'$, x,0,z
   
   (1*) $1$
   
   (2) $2'$, 0,y,0
   
   (3) 1, 0,0,0
   
   (4) $m'$, x,0,z

   (m', 0,0,0)

For (1/2,1/2,0)' + set:

1. $t'$, (1/2,1/2,0)
   
   (1) $t'$, (1/2,1/2,0)
   
   (2) $2$ (0,1/2,0) 1/4,y,0
   
   (3) $t'$, 1/4,1/4,0
   
   (4) $a$ (1/2,0,0) x,1/4,z
   
   (1*) $t'$, (1/2,1/2,0)
   
   (2) $2$ (0,1/2,0) 1/4,y,0
   
   (3) $t'$, 1/4,1/4,0
   
   (4) $a$ (1/2,0,0) x,1/4,z

   (m', 1/2,1/2,0)
Generators selected (1); t(1,0,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>8 j 1</td>
<td>(1) x,y,z [u,v,w] (2) $\bar{x},y,z$ [u,v,w] (3) $\bar{x},y,\bar{z}$ [u,v,w] (4) $x,\bar{y},\bar{z}$ [u,v,w]</td>
</tr>
<tr>
<td>4 i m$'$</td>
<td>x,0,z [u,0,w] $\bar{x},0,\bar{z}$ [u,0,w]</td>
</tr>
<tr>
<td>4 h 2$'$</td>
<td>0,y,1/2 [u,0,w] 0,$\bar{y},1/2$ [u,0,w]</td>
</tr>
<tr>
<td>4 g 2$'$</td>
<td>0,y,0 [u,0,w] 0,$\bar{y},0$ [u,0,w]</td>
</tr>
<tr>
<td>4 f 1$'$</td>
<td>1/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e 1$'$</td>
<td>1/4,1/4,0 [0,0,0] 3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d 2'/m$'$</td>
<td>0,1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 c 2'/m$'$</td>
<td>0,0,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 b 2'/m$'$</td>
<td>0,1/2,0 [u,0,w]</td>
</tr>
<tr>
<td>2 a 2'/m$'$</td>
<td>0,0,0 [u,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] $c_p2'm'$
\[ a^* = a, \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] $p_{2a}2mm$
\[ a^* = b/2, \quad b^* = c_p \]
Origin at x,1/4,0

Along [0,1,0] $p_{2a}211$
\[ a^* = -a/2, \quad b^* = c \]
Origin at 1/4,y,0
Origin at 1 on glide plane c

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
    (1 | 0, 0, 0)
(2) 2 0, y, 1/4
    (2 | 0, 0, 1/2)
(3) 1 0, 0, 0
    (1 | 0, 0, 0)
(4) c (0, 0, 1/2) x, 0, z
    (m | 0, 0, 1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 g 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1)</td>
</tr>
<tr>
<td>2 f 2</td>
<td>1/2,y,1/4 [0,v,0]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 e 2</td>
<td>0,y,1/4 [0,v,0]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 d 1</td>
<td>1/2,0,0 [u,v,w]</td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 c 1</td>
<td>0,1/2,0 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 1</td>
<td>1/2,1/2,0 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>2 a 1</td>
<td>0,0,0 [u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2'mm'</th>
<th>Origin at 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2mg</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>a* = -c</td>
<td>b* = b</td>
<td></td>
</tr>
<tr>
<td>Along [0,1,0]</td>
<td>p_2_a_2_1</td>
<td>Origin at 0,y,1/4</td>
</tr>
<tr>
<td>a* = c/2</td>
<td>b* = a</td>
<td></td>
</tr>
</tbody>
</table>
**Origin**

at 1' on glide plane c1'

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For 1 + set

1. (1, 0, 0, 0)
2. 2, 0, y, 1/4
3. 1, 0, 0, 0
4. c, (0, 0, 1/2), x, 0, z

For 1' + set

1. (1', 0, 0, 0'1)
2. 2', 0, y, 1/4
3. 1, 0, 0, 0
4. c', (0, 0, 1/2), x, 0, z

---

13.2.78 - 1 - 132
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 +</td>
<td>g</td>
<td>1'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 f</td>
<td>1'</td>
<td></td>
<td>1/2,y,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,y,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 e</td>
<td>1'</td>
<td></td>
<td>0,y,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,y,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 d</td>
<td>1'</td>
<td></td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c</td>
<td>1'</td>
<td></td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b</td>
<td>1'</td>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a</td>
<td>1'</td>
<td></td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mm1'  Along [1,0,0]  p2mg1'  Along [0,1,0]  p2111'
\( a^* = a \)  \( b^* = b \)  \( a^* = c/2 \)  \( b^* = a \)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at \( \overline{1} \) on glide plane \( c \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

1. \( 1 \)
   
   \[ (1,0,0,0) \]

2. \( 2' \)
   
   \[ (2',0,y,1/4) \]

3. \( \overline{1}' \)
   
   \[ (3',0,0,0) \]

4. \( c \)
   
   \[ (4,0,0,1/2) \]

\[ (m',0,0,1/2) \]
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>g</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>(1) (x,y,z)</td>
<td>([u,v,w])</td>
</tr>
<tr>
<td>2</td>
<td>f</td>
<td>2'</td>
</tr>
<tr>
<td></td>
<td>1/2,(y,1/4)</td>
<td>([u,0,w])</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>2'</td>
</tr>
<tr>
<td></td>
<td>0,(y,1/4)</td>
<td>([u,0,w])</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>(\bar{1})</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0</td>
<td>([0,0,0])</td>
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<td>2</td>
<td>c</td>
<td>(\bar{1})</td>
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<td>0,1/2,0</td>
<td>([0,0,0])</td>
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<tr>
<td>2</td>
<td>b</td>
<td>(\bar{1})</td>
</tr>
<tr>
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<td>1/2,1/2,0</td>
<td>([0,0,0])</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>(\bar{1})</td>
</tr>
<tr>
<td></td>
<td>0,0,0</td>
<td>([0,0,0])</td>
</tr>
</tbody>
</table>

#### Symmetry of Special Projections

- Along \([0,0,1]\) \(p2mm\)  
  \(a^* = a, b^* = b\)
  Origin at 0,0,z

- Along \([1,0,0]\) \(p2mg\)  
  \(a^* = -c, b^* = b\)
  Origin at x,0,0

- Along \([0,1,0]\) \(p_{2a211}\)  
  \(a^* = c/2, b^* = a\)
  Origin at 0,y,0
Origin at 1 on glide plane c'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
   (1 0,0,0)
(2) 2 0,y,1/4
   (2 0,0,1/2)
(3) 1' 0,0,0
   (1 0,0,0)'
(4) c' (0,0,1/2) x,0,z
   (m 0,0,1/2)'

P2/c' 2/m' Monoclinic
13.4.80 P12/c'1
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

<table>
<thead>
<tr>
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<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>4 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z +1/2 [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 f 2</td>
<td>1/2,y,1/4 [0,v,0]</td>
<td>1/2,y,3/4 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 e 2</td>
<td>0,y,1/4 [0,v,0]</td>
<td>0,y,3/4 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 d 1/2</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 c 1/2</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b 1/2</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 0</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1]  p2m'm'  

a* = a  b* = b  

Origin at 0,0,z

Along [1,0,0]  p2m'g'  

a* = -c  b* = b  

Origin at x,0,0

Along [0,1,0]  p211  

a* = c/2  b* = a  

Origin at 0,y,0
**Origin** at 1 on glide plane c'

**Asymmetric unit**  
\[0 < x < \frac{1}{2}; \quad 0 < y < 1; \quad 0 < z < \frac{1}{2}\]

**Symmetry Operations**

1. 1  \[(0,0,0)\]
2. 2' 0, y, 1/4  \[(2,0,0,1/2)\]
3. 1 0, 0, 0  \[(1,0,0,0)\]
4. c' (0,0,1/2) x, 0, z  \[(m,0,0,1/2)\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

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</thead>
<tbody>
<tr>
<td>4</td>
<td>g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>f 2'</td>
<td>1/2,y,1/4 [u,0,w]</td>
<td>1/2,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>e 2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>d 1</td>
<td>1/2,0,0 [u,v,w]</td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>c 1</td>
<td>0,1/2,0 [u,v,w]</td>
<td>0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 1</td>
<td>1/2,1/2,0 [u,v,w]</td>
<td>1/2,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>a 1</td>
<td>0,0,0 [u,v,w]</td>
<td>0,0,1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mm'  Along [1,0,0] p2'mg'  Along [0,1,0] p2'11
a* = a,  b* = b  a* = -c,  b* = b  a* = c/2  b* = a
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at \( \vec{1} \) on glide plane c

Asymmetric unit \[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{2} \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 0,y,\frac{1}{4} \\
(2) & \quad (0,0,\frac{1}{2}) \\
(3) & \quad \vec{1},0,0 \\
(3) & \quad (0,0,0) \\
(4) & \quad c \\
(4) & \quad (0,0,\frac{1}{2}) \\
(4) & \quad x,0,z \\
(4) & \quad \vec{m},0,0,\frac{1}{2} \\
\end{align*}
\]

For \((1,0,0) + \) set

\[
\begin{align*}
(1) & \quad t' \\
(1) & \quad (1,0,0) \\
(1) & \quad (1,0,0)' \\
(1) & \quad (1,0,0)' \\
(2) & \quad 2' \\
(2) & \quad 1/2,y,1/4 \\
(2) & \quad 1/2,0,1/2 \\
(3) & \quad \vec{1},1/2,0,0 \\
(3) & \quad (1,0,0)' \\
(3) & \quad (1,0,0)' \\
(4) & \quad n' \\
(4) & \quad (1,0,1/2) \\
(4) & \quad x,0,z \\
(4) & \quad \vec{m},1,0,1/2 \\
\end{align*}
\]
Continued 13.6.82  P_{2a}2/c

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 f 2'</td>
<td>1/2,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 e 2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_{2a}2mm  
Along [1,0,0]  p2mg1'  
Along [0,1,0]  p_{2a}211  
a^* = -b  b^* = a_p  
a^* = -c_p  b^* = b  
a^* = -a  b^* = a + c/2  
Origin at 1/2,0,z  
Origin at x,0,0  
Origin at 0,y,1/4
P2\(_b\)2/c

13.7.83

2/m1'

P2\(_b\)12/c1

Monoclinic

Origin at 1 on glide plane c

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 0,0,1/4
(2 | 0,0,0,1/2)

(3) 1 0,0,0
(1 | 0,0,0)

(4) c 0,0,1/2 x,0,z
(m | 0,0,1/2)

For (0,1,0)' + set

(1) t' (0,1,0)
(1 | 0,1,0)'

(2) 2' (0,1,0) 0,y,1/4
(2 | 0,1,1/2)'

(3) 1' 0,1/2,0
(1 | 0,1,0)'

(4) c' (0,0,1/2) x,1/2,z
(m | 0,1,1/2)'

13.7.83 - 1 - 142
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions
Multiplicity,
Wyckoff letter,
Site Symmetry.
Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,1,0)' +</td>
<td></td>
</tr>
<tr>
<td>4 f 2</td>
<td>1/2,y,1/4 [0,v,0]</td>
<td>1/2,y,3/4 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 e 2</td>
<td>0,y,1/4 [0,v,0]</td>
<td>0,y,3/4 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/2,0,0 [u,v,w]</td>
<td>1/2,0,1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 c 1</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b 1</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
<td>0,0,1/2 [u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] \( p_{2a}.2'mm' \)  Along [1,0,0] \( p_{2b}.2mg \)  Along [0,1,0] \( p_{2111}' \)
\( a^* = -b \quad b^* = a_p \) \quad \( a^* = -c_p \quad b^* = b \) \quad \( a^* = c/2 \quad b^* = a \)
Origin at 1/2,0,z  Origin at x,1/2,0  Origin at 0,y,1/4
13.8.84

**PC2/c**

13.8.84

**2/m1’**

**Monoclinic**

- **Origin**: at $\bar{1}$ on glide plane $c$
- **Asymmetric unit**: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$
- **Symmetry Operations**

  For $(0,0,0)$ + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $1$</td>
<td>(2) $2$</td>
<td>(3) $\bar{1}$</td>
<td>(4) $c$</td>
</tr>
<tr>
<td>$(1</td>
<td>0,0,0)$</td>
<td>$0,y,1/4$</td>
<td>$0,0,1/2$</td>
</tr>
<tr>
<td>(2)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

  For $(1,0,0)$ + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $t'$</td>
<td>(2) $2'$</td>
<td>(3) $\bar{1}$</td>
<td>(4) $n'$</td>
</tr>
<tr>
<td>$(1</td>
<td>0,0,0)$</td>
<td>$1/2,y,1/4$</td>
<td>$1/2,0,0$</td>
</tr>
<tr>
<td>(2)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

13.8.84 - 1 - 144
Generators selected  \( (1); t(1,0,0)'; t(0,1,0)'; t(0,0,1); (2); (3). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0) + (1,0,0)' + )</td>
<td></td>
</tr>
<tr>
<td>8 g 1 ((1) x,y,z [u,v,w] ) ((2) \bar{x},y,z+1/2 [\bar{u},v,w] ) ((3) \bar{x},y,z [u,v,w] ) ((4) \bar{x},y,z+1/2 [\bar{u},v,w] )</td>
<td></td>
</tr>
<tr>
<td>4 f 2' ((1/2,y,1/4 [u,0,w] ) (1/2,y,3/4 [u,0,w] )</td>
<td></td>
</tr>
<tr>
<td>4 e 2 ((0,y,1/4 [0,v,0] ) (0,\bar{y},3/4 [0,v,0] )</td>
<td></td>
</tr>
<tr>
<td>4 d 1' ((1/2,0,0 [0,0,0] ) (1/2,0,1/2 [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td>4 c 1' ((0,1/2,0 [0,0,0] ) (0,1/2,1/2 [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td>4 b 1 ((1/2,1/2,0 [u,v,w] ) (1/2,1/2,1/2 [u,\bar{v},w] )</td>
<td></td>
</tr>
<tr>
<td>4 a 1 ((0,0,0 [u,v,w] ) (0,0,1/2 [\bar{u},v,w] )</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] \( p_{c2mm} \)   \( a^* = -b \quad b^* = a_p \)   \( a^* = -c_p \quad b^* = b \)   \( a^* = c/2 \quad b^* = a \)

Origin at 1/2,0,z   Origin at x,0,0   Origin at 0,y,0
**Origin**

at $\overline{1}''$ on glide plane c

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For $(0,0,0)$ + set

1. $1$
2. $2'$ $0, y, 1/4$
3. $1''$ $0,0,0$
4. $c$ $(0,0,1/2)$ $x,0,z$

For $(0,1,0)''$ + set

1. $t'$ $(0,1,0)$
2. $2$ $(0,1,0)$ $0, y, 1/4$
3. $1''$ $0,1/2,0$
4. $c'$ $(0,0,1/2)$ $x,1/2,z$

---

P2b$2'/c$

2/m1'

Monoclinic

P2b12'/c1

13.9.85
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 f 2'</td>
<td>1/2,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 e 2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a*2mm  
Along [1,0,0] p2b*2mg  
Along [0,1,0] p2111’

\( a^* = -b \)  \( b^* = a_p \)  
\( a^* = -c_p \)  \( b^* = b \)  
\( a^* = c/2 \)  \( b^* = a \)  

Origin at 1/2,0,z  
Origin at x,1/2,0  
Origin at 0,y,1/4
Origin at $1$

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

$(1) \quad 1 \quad (2) \quad (0,1/2,0) \quad 0,y,1/4 \quad (3) \quad \overline{1} \quad 0,0,0 \quad (4) \quad c \quad (0,0,1/2) \quad x,1/4,z$

$(1 \quad 0,0,0) \quad (2 \quad 0,1/2,1/2) \quad (3 \quad 0,0,0) \quad (4 \quad m \quad 0,1/2,1/2)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>2 d 1/2</td>
<td>1/2,0,0</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>2 c 0</td>
<td>0,1/2,0</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>2 b 1/2</td>
<td>1/2,1/2,0</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>2 a 0</td>
<td>0,0,0</td>
<td>[u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2'mg'</th>
<th>Along [1,0,0] p2'gg'</th>
<th>Along [0,1,0] p2c-211</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{a}^* = -\mathbf{b} ) ( \mathbf{b}^* = \mathbf{a}_p )</td>
<td>( \mathbf{a}^* = \mathbf{b} ) ( \mathbf{b}^* = \mathbf{c}_p )</td>
<td>( \mathbf{a}^* = \mathbf{c}/2 ) ( \mathbf{b}^* = \mathbf{a} )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,1/4</td>
</tr>
</tbody>
</table>
Origin at $1$'

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

For $1$ + set

(1) $1$

(1) $0,0,0$

(2) $0,1/2,0$ $0,y,1/4$

(2) $x,0,1/2,1/2$

(3) $1$ $0,0,0$

(3) $0,0,0$

(4) $c$ $x,1/4,z$

(4) $m_{ij}$ $0,0,1/2,1/2$

For $1'$ + set

(1) $1$

(1) $0,0,0$

(2) $0,1/2,0$ $0,y,1/4$

(2) $x,0,1/2,1/2$

(3) $1$ $0,0,0$

(3) $0,0,0$

(4) $c'$ $x,1/4,z$

(4) $m_{ij}$ $0,0,1/2,1/2$
Generators selected  
(1); t(1,0,0); t(0,0,1); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
<th>1+</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 11' (1) x,y,z [0,0,0]</td>
<td>(2) x,y+1/2,z+1/2 [0,0,0]</td>
<td>(3) x,y,z [0,0,0]</td>
<td>(4) x,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 d 1' 1/2,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 1' 0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b 1' 1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a 1' 0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg1'  
\[a^* = -b \quad b^* = a_p\]
Origin at 0,0,z

Along [1,0,0] p2gg1'  
\[a^* = b \quad b^* = c_p\]
Origin at x,0,0

Along [0,1,0] p2111'  
\[a^* = c/2 \quad b^* = a\]
Origin at 0,y,0
Origin at \( \frac{1}{4} \)

Asymmetric unit: \( 0 \leq x \leq 1; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1 \)

Symmetry Operations:

1. \( \text{1} \)
   \( (0,0,0) \)

2. \( \text{2}' \) \((0,1/2,0)\) \(0;y,1/4\)

3. \( \text{1}' \) \((0,0,0)\)

4. \( c \) \((0,0,1/2)\) \(x,1/4,z\)

\( (m) \) \((0,1/2,1/2)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 d T'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c T'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b T'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a T'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg  
Along [1,0,0] p2gg  
Along [0,1,0] p2a'211

a* = -b  
b* = a  
a* = c/a  
b* = a  

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at $1'$

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) $1$

(2) $2 (0,1/2,0) \quad 0,y,1/4$

(3) $1' \quad 0,0,0$

(4) $c' (0,0,1/2) \quad x,1/4,z$

\[ (1 | 0,0,0) \]

\[ (2, y | 0,1/2,1/2) \]

\[ (3, y' | 0,0,0) \]

\[ (m, 0,1/2,1/2) \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 d 1/2,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'g'
- \( \mathbf{a}^* = -\mathbf{b} \)
- \( \mathbf{b}^* = \mathbf{a}_p \)
- Origin at 0,0,z

Along [1,0,0] p2g'g'
- \( \mathbf{a}^* = \mathbf{b} \)
- \( \mathbf{b}^* = \mathbf{c}_p \)
- Origin at x,0,0

Along [0,1,0] p211
- \( \mathbf{a}^* = \mathbf{c}/2 \)
- \( \mathbf{b}^* = \mathbf{a} \)
- Origin at 0,y,0
Origin at \( \bar{1} \)

Asymmetric unit \( 0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \)

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2' \quad (0,1/2,0) \quad 0,y,1/4 \\
(3) & \quad \bar{1} \quad 0,0,0 \\
(4) & \quad c' \quad (0,0,1/2) \quad x,1/4,z \\
(5) & \quad m \quad (0,1/2,1/2)' \end{align*}
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 d</td>
<td>1/2,0,0 [u,v,w]</td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 c</td>
<td>0,1/2,0 [u,v,w]</td>
<td>0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 b</td>
<td>1/2,1/2,0 [u,v,w]</td>
<td>1/2,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 a</td>
<td>0,0,0 [u,v,w]</td>
<td>0,0,1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p2'm'g  
Along [1,0,0] p2'gg'  
Along [0,1,0] p2'11

- \(a^* = a, \quad b^* = b\)  
- \(a^* = -c, \quad b^* = b\)  
- \(a^* = c/2, \quad b^* = a\)  
- Origin at 0,0,z  
- Origin at x,0,0  
- Origin at 0,y,1/4
Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq 1; \enspace 0 \leq y \leq 1/4; \enspace 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

$(1) \bar{1} \quad (2) (0,1/2,0) \quad 0,y,1/4 \quad (3) \bar{1} \quad 0,0,0 \quad (4) c \quad (0,0,1/2) \quad x,1/4,z$

$(2) (0,1/2,0) \quad (1/2,y,1/4)$

$(3) \bar{1} \quad 0,0,0 \quad (1 \bar{1},0,0,0)$

$(4) c \quad (0,0,1/2) \quad x,1/4,z \quad (m,0,1/2,1/2)$

For $(1,0,0)' +$ set

$(1) t' \quad (1,0,0) \quad (2) 2' (0,1/2,0) \quad 1/2,y,1/4 \quad (3) \bar{1}' \quad 1/2,0,0 \quad (4) n' \quad (1,0,1/2) \quad x,1/4,z$

$(1 \bar{1},0,0)' \quad (2 \bar{1},1/2,1/2)'$

$(3) \bar{1}' \quad 1/2,0,0 \quad (1 \bar{1},1,0,0)'$

$(4) n' \quad (1,0,1/2) \quad x,1/4,z \quad (m,1,1/2,1/2)'$
Continued 14.6.91 P2a21/c

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicities, Wyckoff letters, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2g*2mg
  - \( \mathbf{a}^* = -\mathbf{b}, \mathbf{b}^* = \mathbf{a} \)
  - Origin at 1/2,0,z

- Along [1,0,0] p2gg1'
  - \( \mathbf{a}^* = \mathbf{b}, \mathbf{b}^* = \mathbf{c} \)
  - Origin at x,0,0

- Along [0,1,0] p2a211
  - \( \mathbf{a}^* = \mathbf{c}/2, \mathbf{b}^* = \mathbf{a} + \mathbf{c}/2 \)
  - Origin at 0,y,1/4
Origin at 1 on glide plane c

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set
(1) 1
(1 | 0,0,0)
(2) 2 0,y,1/4
(2 | 0,0,1/2)
(3) 1 0,0,0
(1 | 0,0,0)
(4) c (0,0,1/2) x,0,z
(m | 0,0,1/2)

For (1/2,1/2,0) + set
(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)
(2) 2 (0,1/2,0) 1/4,y,1/4
(2 | 1/2,1/2,1/2)
(3) 1 1/4,1/4,0
(1 | 1/2,1/2,0)
(4) n (1/2,0,1/2) x,1/4,z
(m | 1/2,1/2,1/2)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

<table>
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<tr>
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</tr>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z +1/2 [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 e 2</td>
<td>0,y,1/4 [0,v,0] 0,y,3/4 [0,v,0]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/4,1/4,1/2[u,v,w] 3/4,1/4,0 [u,v,w]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>1/4,1/4,0 [u,v,w] 3/4,1/4,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,1/2,0 [u,v,w] 0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w] 0,0,1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2'm'm' Along [1,0,0] p2'm'g Along [0,1,0] P2a-211
\[ a^* = -b \quad b^* = a_p \]
\[ a^* = -c_p \quad b^* = b/2 \]
\[ a^* = c/2 \quad b^* = a/2 \]

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
C2/c1' 2/m1' Monoclinic

15.2.93 C12/c11'

Origin at 1' on glide plane c1'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 0,0,0
(1 0,0,0)

(2) 2 0,y,1/4 (2 0,0,1/2)

(3) 1 0,0,0 (3 0,0,0)

(4) c (0,0,1/2) x,0,z

For (1/2,1/2,0) + set

(1) t 1/2,1/2,0 (1 1/2,1/2,0)

(2) 2 0,1/2,0 1/4,y,1/4 (2 1/2,1/2,1/2)

(3) 1 1/4,1/4,0 (3 1/2,1/2,0)

(4) n (1/2,0,1/2) x,1/4,z

For (0,0,0)' + set

(1) 1' 0,0,0 (1 0,0,0)

(2) 2' 0,y,1/4 (2 0,0,1/2)

(3) 1' 0,0,0 (3 0,0,0)

(4) c' (0,0,1/2) x,0,z

For (1/2,1/2,0)' + set

(1) t' 1/2,1/2,0 (1 1/2,1/2,0)

(2) 2' 0,1/2,0 1/4,y,1/4 (2 1/2,1/2,1/2)

(3) 1' 1/4,1/4,0 (3 1/2,1/2,0)

(4) n' (1/2,0,1/2) x,1/4,z

15.2.93 - 1 - 162
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) +</td>
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</tr>
<tr>
<td>8 f 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) (\bar{x},y,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) (\bar{x},y,z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) (x,y,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td>4 e 21'</td>
<td>0,y,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 d (\bar{1})'</td>
<td>1/4,1/4,1/2[0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c (\bar{1})'</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b (\bar{1})'</td>
<td>0,1/2,0 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a (\bar{1})'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1] c2mm1'               Along [1,0,0] p2mg1'               Along [0,1,0] p2111'  
\(a^* = a, \quad b^* = b\)        \(a^* = -c, \quad b^* = b/2\)        \(a^* = c/2, \quad b^* = a/2\)  
Origin at 0,0,z                    Origin at x,0,0                    Origin at 0,y,0
C2'/c 2'/m Monoclinic

15.3.94  C12'/c1

Origin  at 1' on glide plane c

Asymmetric unit  0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2' 0,y,1/4
   (2',0,0,1/2)
(3) 1' 0,0,0
(4) c 0,0,1/2
(1)' 0,0,0
(2)' y 0,0,1/2
(3)' 0,0,0
(4)' m 0,0,1/2

For (1/2,1/2,0) + set

(1) t 1/2,1/2,0
(2) 2' (0,1/2,0) 1/4,y,1/4
   (2',1/2,1/2,1/2)
(3) 1' 1/4,1/4,0
(4) n (1/2,0,1/2) x,1/4,z
(1)' 1/2,1/2,0
(2)' 1/2,1/2,1/2
(3)' 1/4,1/4,0
(4)' m 1/2,1/2,1/2
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e '2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 d '1)'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c '1)'</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b '1)'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a '1)'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] c2mm  
  \( \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \)
- Along [1,0,0] p2mg  
  \( \mathbf{a}^* = -\mathbf{c}, \mathbf{b}^* = \mathbf{b}/2 \)
- Along [0,1,0] \( \mathbf{p}_{\mathbf{2a},21\overline{1}} \)  
  \( \mathbf{a}^* = \mathbf{c}/2, \mathbf{b}^* = \mathbf{a}/2 \)

Origin at 0,0,0  
Origin at x,0,0  
Origin at 0,y,0
Origin at $\overline{1}$ on glide plane $c'$

Asymmetric unit $\ 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

$(1) \ 1$
$(1 \ | \ 0,0,0)$

$(2) \ 2 \ 0,y,1/4$
$(2 \ | \ 0,0,1/2)$

$(3) \ \overline{1}^{'} \ 0,0,0$
$(1 \ | 0,0,0)^{'}$

$(4) \ c' \ (0,0,1/2) \ x,0,z$
$(m_{y} | 0,0,1/2)^{'}$

For $(1/2,1/2,0)$ + set

$(1) \ t \ (1/2,1/2,0)$
$(1 \ | 1/2,1/2,0)$

$(2) \ 2 \ (0,1/2,0) \ 1/4,y,1/4$
$(2 \ | 1/2,1/2,1/2)$

$(3) \ \overline{1}^{'} \ 1/4,1/4,0$
$(1 \ | 1/2,1/2,0)^{'}$

$(4) \ n' \ (1/2,0,1/2) \ x,1/4,z$
$(m_{y} | 1/2,1/2,1/2)^{'}$
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>8 f 1</td>
<td>((0,0,0)) + ((1/2,1/2,0)) +</td>
<td>((1)) (</td>
<td>x,y,z</td>
</tr>
<tr>
<td>4 e 2</td>
<td>0, 1/4 [0, v, 0]</td>
<td>((3)) (</td>
<td>x,y,z</td>
</tr>
<tr>
<td>4 d (\bar{1})</td>
<td>1/4, 1/4, 1/2 [0, 0, 0]</td>
<td>3/4, 1/4, 0 [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>4 c (\bar{1})</td>
<td>1/4, 1/4, 0 [0, 0, 0]</td>
<td>3/4, 1/4, 1/2 [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>4 b (\bar{1})</td>
<td>0, 1/2, 0 [0, 0, 0]</td>
<td>0, 1/2, 1/2 [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>4 a (\bar{1})</td>
<td>0, 0, 0 [0, 0, 0]</td>
<td>0, 0, 1/2 [0, 0, 0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \(c2m'm'\) \(a^* = a, \ b^* = b\) Origin at 0, 0, z
Along \([1,0,0]\) \(p2m'g'\) \(a^* = -c, \ b^* = b/2\) Origin at x, 0, 0
Along \([0,1,0]\) \(p211\) \(a^* = c/2, \ b^* = a/2\) Origin at 0, y, 0
Origin at \( \bar{1} \) on glide plane \( c' \)

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

(1) \( \bar{1} \) \( (1 \mid 0,0,0) \)
(2) \( 2' \) \( 0, y, 1/4 \)
(3) \( \bar{1} \) \( 0,0,0 \)
(4) \( c' \) \( (0,0,1/2) \) \( x,0,z \)

For \((1/2,1/2,0) + \text{set}\)

(1) \( t \) \( (1/2,1/2,0) \)
(2) \( 2' \) \( (0,1/2,0) \) \( 1/4,y,1/4 \)
(3) \( \bar{1} \) \( 1/2,1/2,0 \)
(4) \( n' \) \( (1/2,0,1/2) \) \( x,1/4,z \)

**C2'/c'**

15.5.96

**2'/m'**

C12'/c'1

**Monoclinic**
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(0,0,0)</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e 2'</td>
<td>(0,0,0)</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>(1/4,1/4,0)</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>(1/4,1/4,0)</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>(0,1/2,0)</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>(0,0,0)</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2'mm'  Along [1,0,0]  p2'mg'  Along [0,1,0]  p2'11

a' = a  b' = b  a' = -c  b' = b/2  a' = c/2  b' = a/2

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at $\tilde{1}$ on glide plane $c$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) + \text{ set}$

(1) $1$
    \( (1|0,0,0) \)

(2) $2$  $0, y, 1/4$
    \( (2|0,0,1/2) \)

(3) $\tilde{1}$  $0,0,0$
    \( (\tilde{1}|0,0,0) \)

(4) $c$  $(0,0,1/2)$  $x,0,z$
    \( (m,0,0,1/2) \)

For $(1/2,1/2,0)' + \text{ set}$

(1) $\tilde{1}'$  $(1/2,1/2,0)$
    \( (1|1/2,1/2,0') \)

(2) $2'$  $(0,1/2,0)$  $1/4, y, 1/4$
    \( (2|1/2,1/2,1/2') \)

(3) $\tilde{1}'$  $1/4,1/4,0$
    \( (\tilde{1}|1/2,1/2,0') \)

(4) $n'$  $(1/2,0,1/2)$  $x,1/4,z$
    \( (m,1/2,1/2,1/2') \)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t (1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) + (1/2,1/2,0)° +</td>
</tr>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e 2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/4,1/4,1/2[0,0,0]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin</th>
<th>a° = -b° b° = a°</th>
<th>a° = -c° b° = b/2</th>
<th>a° = c/2 b° = a/2 + c/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>c° 2'mm'</td>
<td>p° 2b° 2mg</td>
<td>p° 2a° 211</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along [0,1,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin at \( \mathbf{1}^\prime \) on glide plane \( c \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

For \((0,0,0) + \) set

(1) \(1\)
(1) \( \mathbf{1} \)
(0,0,0)
(2) \(2^\prime \) \(0,y,1/4\)
(2) \( 2^\prime \)
(0,0,1/2)
(3) \(1^\prime \)
(3) \( \mathbf{1}^\prime \)
(0,0,0)
(4) \(c\)
(4) \(c\)
(0,0,1/2)

For \((1/2,1/2,0)^\prime + \) set

(1) \(t^\prime \)
(1) \( t^\prime \)
(1/2,1/2,0)
(1) \( t^\prime \)
(1/2,1/2,0)
(2) \( 2 \) \(0,1/2,0\)
(2) \( 2 \)
(0,1/2,0)
(3) \( \mathbf{1}^\prime \)
(3) \( \mathbf{1}^\prime \)
(1/4,1/4,0)
(4) \(n^\prime \)
(4) \( n^\prime \)
(1/2,0,1/2)

(1/2,1/2,0)^\prime
(1/2,1/2,0)^\prime
(1/2,1/2,1/2)
(1/2,1/2,1/2)

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Generators selected \( t(1,0,0); t(0,0,1); t(1/2,1/2,0)^*; (2); (3) \).

<table>
<thead>
<tr>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
</tr>
<tr>
<td>((0,0,0) + (1/2,1/2,0)^* + )</td>
</tr>
<tr>
<td>8 f 1 ((1) x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>4 e 2' 0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 d 1/4,1/4,1/2[u,v,w]</td>
</tr>
<tr>
<td>4 c 1/4,1/4,0 [u,v,w]</td>
</tr>
<tr>
<td>4 b 0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along ( [0,0,1] )</th>
<th>( c_p 2\text{mm} )</th>
<th>Along ( [1,0,0] )</th>
<th>( p_{21b} 2\text{mg} )</th>
<th>Along ( [0,1,0] )</th>
<th>( p_{2a} 211 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^<em>=a ) ( b^</em>=b )</td>
<td>( a^<em>=-c ) ( b^</em>=b/2 )</td>
<td>( a^<em>=c/2 ) ( b^</em>=a/2 + c/2 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,( z )</td>
<td>Origin at ( x,0,0 )</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Asymmetric unit: $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations:

1. $1$
   - $x, y, z$
2. $2x, y, 0$
3. $2x, 0, z$
4. $2x, 0, 0$

Origin at 222

P222

222

Orthorhombic
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>u 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>t ..2 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>s ..2 0,1/2,z [0,0,w] 0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>r ..2 1/2,0,z [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>q ..2 0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>p ..2 1/2,y,1/2 [0,v,0] 1/2,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>o ..2 1/2,y,0 [0,v,0] 1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>n ..2 0,y,1/2 [0,v,0] 0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>m ..2 0,y,0 [0,v,0] 0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>l ..2 x,1/2,1/2 [u,0,0] x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>k ..2 x,1/2,0 [u,0,0] x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>j ..2 x,0,1/2 [u,0,0] x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>i ..2 x,0,0 [u,0,0] x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>h 222 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>g 222 0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>f 222 1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>e 222 1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>d 222 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>c 222 0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>b 222 1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a 222 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'  Along [1,0,0] p2m'm'  Along [0,1,0] p2m'm'

**a** = **a**  **b** = **b**  **a** = **b**  **b** = **c**  **a** = **c**  **b** = **a**

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For 1 + set

1. \( 1 \)
   (1) \( 1 \)
   (2) \( 2 \ 0,0,z \)
   (3) \( 2 \ 0,y,0 \)
   (4) \( 2 \ x,0,0 \)

   (1\* \( 1 \ 0,0,0 \))
   (2\* \( 2 \ 0,0,0 \))
   (3\* \( 2 \ 0,0,0 \))
   (4\* \( 2 \ 0,0,0 \))

For 1' + set

1'. \( 1' \)
   (1') \( 1' \)
   (2') \( 2' \ 0,0,z \)
   (3') \( 2' \ 0,y,0 \)
   (4') \( 2' \ x,0,0 \)

   (1\* \( 0,0,0 \))
   (2\* \( 0,0,0 \))
   (3\* \( 0,0,0 \))
   (4\* \( 0,0,0 \))

Origin at 2221'
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 u 11'</td>
<td>x,y,z [0,0,0]</td>
<td>( \bar{x},y,z [0,0,0] )</td>
</tr>
<tr>
<td>2 t .21'</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,( \bar{z} ) [0,0,0]</td>
</tr>
<tr>
<td>2 s .21'</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,( \bar{z} ) [0,0,0]</td>
</tr>
<tr>
<td>2 r .21'</td>
<td>1/2,0,z [0,0,0]</td>
<td>1/2,0,( \bar{z} ) [0,0,0]</td>
</tr>
<tr>
<td>2 q .21'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,( \bar{z} ) [0,0,0]</td>
</tr>
<tr>
<td>2 p .21'</td>
<td>1/2,y,1/2 [0,0,0]</td>
<td>1/2,( \bar{y} ),1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 o .21'</td>
<td>1/2,y,0 [0,0,0]</td>
<td>1/2,( \bar{y} ),0 [0,0,0]</td>
</tr>
<tr>
<td>2 n .21'</td>
<td>0,y,1/2 [0,0,0]</td>
<td>0,( \bar{y} ),1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 m .21'</td>
<td>0,y,0 [0,0,0]</td>
<td>0,( \bar{y} ),0 [0,0,0]</td>
</tr>
<tr>
<td>2 l .21'</td>
<td>x,1/2,1/2 [0,0,0]</td>
<td>x,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 k .21'</td>
<td>x,1/2,0 [0,0,0]</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 j .21'</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 i .21'</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>1 h 2221'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>( \bar{x},\bar{y},\bar{z} [0,0,0] )</td>
</tr>
<tr>
<td>1 g 2221'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>( \bar{x},y,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>1 f 2221'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>( \bar{x},0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>1 e 2221'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>( \bar{x},y,\bar{z} [0,0,0] )</td>
</tr>
<tr>
<td>1 d 2221'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>( \bar{x},0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>1 c 2221'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>( \bar{x},1/2,0 [0,0,0] )</td>
</tr>
<tr>
<td>1 b 2221'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>( \bar{x},1/2,0 [0,0,0] )</td>
</tr>
<tr>
<td>1 a 2221'</td>
<td>0,0,0 [0,0,0]</td>
<td>( \bar{x},0,0 [0,0,0] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [0,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a )</td>
<td>( b^* = b )</td>
<td>( a^* = b )</td>
<td>( b^* = c )</td>
<td>( a^* = c )</td>
<td>( b^* = a )</td>
</tr>
</tbody>
</table>
Origin at 2'2'2

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
   (1|0,0,0)
(2) 2 0,0,z
   (2|0,0,0)
(3) 2' 0,y,0
   (2'1|0,0,0)
(4) 2' x,0,0
   (2'2|0,0,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 u 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 t ..2</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 s ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 r ..2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 q ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 p ..2'</td>
<td>1/2, y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 o ..2'</td>
<td>1/2, y,0 [u,0,w]</td>
</tr>
<tr>
<td>2 n ..2'</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 m ..2'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>2 l 2'..</td>
<td>x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 k 2'..</td>
<td>x,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td>2 j 2'..</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 i 2'..</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>1 h 2'2'2</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 g 2'2'2</td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 f 2'2'2</td>
<td>1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 e 2'2'2</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>1 d 2'2'2</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 c 2'2'2</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>1 b 2'2'2</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>1 a 2'2'2</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1]  p2mm  
  \( a^* = a \quad b^* = b \)
  Origin at 0,0,z

- Along [1,0,0]  p2'2'm  
  \( a^* = -c \quad b^* = b \)
  Origin at x,0,0

- Along [0,1,0]  p2'2'm'  
  \( a^* = c \quad b^* = a \)
  Origin at 0,y,0
**Orthorhombic**

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

For \((0,0,0) +\) set

1. \((1) \ 1\ 0,0,0\)
2. \((2) \ 2 \ 0,0,z\)
3. \((3) \ 2 \ 0,y,0\)
4. \((4) \ 2 \ x,0,0\)

For \((1,0,0)'+\) set

1. \((1) \ t'(1,0,0)\)
2. \((2) \ 2' \ 1/2,0,z\)
3. \((3) \ 2' \ 1/2,y,0\)
4. \((4) \ 2'(1,0,0) \ x,0,0\)

**Origin** at 222
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3) \).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 8 ) u 1 ( (1) ) ( x,y,z ) [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>( 4 ) t ( .2' ) ( 1/2,1/2,z ) [u,v,0]</td>
<td>(1,0,0)'' +</td>
</tr>
<tr>
<td>( 4 ) s ( .2 ) ( 0,1/2,z ) [0,0,w]</td>
<td>(0,v,w)</td>
</tr>
<tr>
<td>( 4 ) r ( .2' ) ( 1/2,0,z ) [u,v,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) q ( .2 ) ( 0,0,z ) [0,0,w]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) p ( .2' ) ( 1/2,y,1/2 ) [u,w]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) o ( .2' ) ( 1/2,y,0 ) [u,w]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) n ( .2 ) ( 0,y,1/2 ) [0,v,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) m ( .2 ) ( 0,y,0 ) [0,v,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) l ( 2.. ) ( x,1/2,1/2 ) [u,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) k ( 2.. ) ( x,1/2,0 ) [u,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) j ( 2.. ) ( x,0,1/2 ) [0,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 4 ) i ( 2.. ) ( x,0,0 ) [0,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) h ( 22'2' ) ( 1/2,1/2,1/2 ) [u,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) g ( 222 ) ( 0,1/2,1/2 ) [0,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) f ( 22'2' ) ( 1/2,0,1/2 ) [u,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) e ( 22'2' ) ( 1/2,1/2,0 ) [u,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) d ( 222 ) ( 0,0,1/2 ) [0,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) c ( 222 ) ( 0,1/2,0 ) [0,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) b ( 22'2' ) ( 1/2,0,0 ) [u,0,0]</td>
<td>(u,v,0)</td>
</tr>
<tr>
<td>( 2 ) a ( 222 ) ( 0,0,0 ) [0,0,0]</td>
<td>(u,v,0)</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: \( p_{2a}2m'm' \)
  - \( a^* = a \) \( b^* = b \)
  - Origin at 0,0,z

- **Along [1,0,0]**: \( p2mm1' \)
  - \( a^* = b \) \( b^* = c \)
  - Origin at x,0,0

- **Along [0,1,0]**: \( p_{2a}2m'm' \)
  - \( a^* = -a \) \( b^* = c \)
  - Origin at 0,y,0
Origin at 222

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

(1) $I$
(2) $2 \ 0,0,z$
(3) $2 \ 0,y,0$
(4) $2 \ x,0,0$

For $(1,0,0)'$ + set

(1) $t' \ (1,0,0)$
(2) $2' \ 1/2,0,z$
(3) $2' \ 1/2,y,0$
(4) $2' \ (1,0,0) \ x,0,0$

(1) $t' \ (1,0,0)'$
(2) $2' \ 1,0,0')$
(3) $2' \ (1,0,0)'$
(4) $2' \ (1,0,0)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1,0,0)' +</td>
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</tr>
<tr>
<td>8 u 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 t ..2 1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 s ..2' 0,1/2,z [u,v,0]</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 r ..2' 1/2,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
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<tr>
<td>4 q ..2 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 p ..2' 1/2,y,1/2 [u,0,0]</td>
<td>1/2,y,1/2 [u,0,0]</td>
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<tr>
<td>4 o ..2' 1/2,y,0 [u,0,0]</td>
<td>1/2,y,0 [u,0,0]</td>
</tr>
<tr>
<td>4 n ..2 0,y,1/2 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 m ..2 0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 l 2'. x,1/2,1/2 [0,v,w]</td>
<td>x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 k 2'. x,1/2,0 [0,v,w]</td>
<td>x,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td>4 j 2.. x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 i 2.. x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2 h 2'2' 1/2,1/2,1/2 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 g 2'2' 0,1/2,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 f 2'2' 1/2,0,1/2 [u,0,0]</td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 e 2'2' 1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 d 222 0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 2'2' 0,1/2,0 [0,v,0]</td>
<td>0,1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>2 b 22' 1/2,0,0 [u,0,0]</td>
<td>1/2,0,0 [u,0,0]</td>
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<tr>
<td>2 a 222 0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_c2mm
\[ a^* = a \quad b^* = b \]
Origin at 1/2,1/2,z

Along [1,0,0] p2mm1'
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [0,1,0] p2mm1'
\[ a^* = c \quad b^* = a \]
Origin at 0,y,0
Origin at 222

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2z 0,0,z
(2z | 0,0,0)

(3) 2y 0,y,0
(2y | 0,0,0)

(4) 2x x,0,0
(2x | 0,0,0)

For (1,0,0)’ + set

(1) t’ (1,0,0)
(1 | 1,0,0)’

(2) 2’ 1/2,0,z
(2’ | 1,0,0)’

(3) 2’ 1/2,y,0
(2’ | 1,0,0)’

(4) 2’ (1,0,0) x,0,0
(2’ | 1,0,0)’
Generators selected \( t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0) +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 u 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>( \bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}] )</td>
</tr>
<tr>
<td>4 t .2</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,\bar{z} [0,0,w]</td>
</tr>
<tr>
<td>4 s .2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>0,1/2,\bar{z} [\bar{u},\bar{v},0]</td>
</tr>
<tr>
<td>4 r .2'</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,0,\bar{z} [\bar{u},\bar{v},0]</td>
</tr>
<tr>
<td>4 q .2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,\bar{z} [0,0,\bar{w}]</td>
</tr>
<tr>
<td>4 p .2</td>
<td>1/2,y,1/2 [0,v,0]</td>
<td>1/2,\bar{y},1/2 [0,\bar{v},0]</td>
</tr>
<tr>
<td>4 o .2'</td>
<td>1/2,y,0 [u,0,w]</td>
<td>1/2,\bar{y},0 [u,0,\bar{w}]</td>
</tr>
<tr>
<td>4 n .2'</td>
<td>0,y,1/2 [u,0,w]</td>
<td>0,\bar{y},1/2 [\bar{u},0,w]</td>
</tr>
<tr>
<td>4 m .2</td>
<td>0,y,0 [0,v,0]</td>
<td>0,\bar{y},0 [0,\bar{v},0]</td>
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<tr>
<td>4 l .2..</td>
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<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 k .2'..</td>
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<td>x,1/2,0 [0,v,\bar{w}]</td>
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<tr>
<td>4 j .2'..</td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,\bar{v},w]</td>
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<td>4 i .2..</td>
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<td>x,0,0 [u,0,0]</td>
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<td>2 h 222</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 g 222'</td>
<td>0,1/2,1/2 [u,0,0]</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 f 2'2'</td>
<td>1/2,0,1/2 [0,v,0]</td>
<td>1/2,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>2 e 2'2'</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 d 2'2'</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c 2'2'</td>
<td>0,1/2,0 [0,v,0]</td>
<td>0,1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>2 b 222'</td>
<td>1/2,0,0 [u,0,0]</td>
<td>1/2,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2 a 222</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- **Along [0,0,1]** \( \text{p}2\text{mm}1' \)
  \( a^* = a \quad b^* = b \)
  Origin at 0,0,z

- **Along [1,0,0]** \( \text{p}2\text{mm}1' \)
  \( a^* = b \quad b^* = c \)
  Origin at x,0,0

- **Along [0,1,0]** \( \text{p}2\text{mm}1' \)
  \( a^* = c \quad b^* = a \)
  Origin at 0,y,0
P_{2c22'2'}

16.7.105

P_{2c22'2'}

Orthorhombic

Origin at 22'2'

Asymmetric unit
0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) \text{1}
(1|0,0,0)

(2) 2' 0,0,z
(2_z|0,0,0)'

(3) 2' 0,y,0
(2_y|0,0,0)'

(4) 2 x,0,0
(2_x|0,0,0)

For (0,0,1)' + set

(1) t' (0,0,1)
(1|0,0,1)'

(2) 2 (0,0,1) 0,0,z
(2_z|0,0,1)

(3) 2 0,y,1/2
(2_y|0,0,1/2)

(4) 2' x,0,1/2
(2_x|0,0,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) + (0,0,1)′ +</td>
</tr>
<tr>
<td>8 u 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 t .2′</td>
<td>1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 s .2′</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 r .2′</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 q .2′</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 p .2′</td>
<td>1/2,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 o .2′</td>
<td>1/2,y,0 [u,0,0]</td>
</tr>
<tr>
<td>4 n .2′</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 m .2′</td>
<td>0,y,0 [u,0,0]</td>
</tr>
<tr>
<td>4 l 2′..</td>
<td>x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 k 2′.</td>
<td>x,1/2,0 [u,0,0]</td>
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<tr>
<td>4 j 2′.</td>
<td>x,0,1/2 [0,v,w]</td>
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<tr>
<td>4 i 2′.</td>
<td>x,0,0 [u,0,0]</td>
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<td>2 h 2′2′</td>
<td>1/2,1/2,1/2 [0,v,0]</td>
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<td>2 g 2′2′</td>
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<td>2 d 2′2′</td>
<td>0,0,1/2 [0,v,0]</td>
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<tr>
<td>2 c 2′2′</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>2 b 2′2′</td>
<td>1/2,0,0 [u,0,0]</td>
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<tr>
<td>2 a 2′2′</td>
<td>0,0,0 [u,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1′  
Along [1,0,0] p2a2mm  
Along [0,1,0] p2a2mm

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z  
Origin at x,0,0  
Origin at 1/2,y,0
Origin at 21_2,

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

1. $1$
   
   2. $(0,0,1/2); \quad 0,0,z$
   
   3. $2 \quad 0,y,1/4$
   
   4. $x,0,0$
   
   (Note: The operations are represented by arrows and points in the diagram.)
Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
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<td>(1) x,y,z [u,v,w] (2) x,y,z+1/2 [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 d .2.</td>
<td>1/2,y,1/4 [0,v,0] 1/2,y,3/4 [0,v,0]</td>
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<tr>
<td>2 c .2.</td>
<td>0,y,1/4 [0,v,0] 0,y,3/4 [0,v,0]</td>
</tr>
<tr>
<td>2 b 2..</td>
<td>x,1/2,0 [u,0,0] x,1/2,1/2 [u,0,0]</td>
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<tr>
<td>2 a 2..</td>
<td>x,0,0 [u,0,0] x,0,1/2 [u,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'p'
\(a^* = a\) \(b^* = b\) \(c^* = c\) \(b^* = b\)
Origin at 0,0,z

Along [1,0,0] p2m'g'
\(a^* = c\) \(b^* = a\)
Origin at x,0,0

Along [0,1,0] p2m'g'
\(a^* = a\) \(b^* = b\)
Origin at 0,y,1/4
Origin at 212,1'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For 1 + set

1. \( (1) \ 1 \quad (1 \ 0,0,0) \)
2. \( (2) \ 2 \ 0,0,1/2 \quad 0,0,z \)
   \( (2_z \ 0,0,1/2) \)
3. \( (3) \ 2 \ 0,y,1/4 \quad (2_y \ 0,0,1/2) \)
4. \( (4) \ 2 \ x,0,0 \quad (2_x \ 0,0,0) \)

For 1' + set

1. \( (1') \ 1' \quad (1' \ 0,0,0) \)
2. \( (2) \ 2' \ 0,0,1/2 \quad 0,0,z \)
   \( (2_z' \ 0,0,1/2) \)
3. \( (3) \ 2' \ 0,y,1/4 \quad (2_y' \ 0,0,1/2) \)
4. \( (4) \ 2' \ x,0,0 \quad (2_x' \ 0,0,0) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
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<tr>
<td>4 e 11'</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
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<td>2 d .2.1'</td>
<td>[0,0,0]</td>
<td>1/2,y,1/4</td>
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</tr>
<tr>
<td>2 c .2.1'</td>
<td>[0,0,0]</td>
<td>0,y,1/4</td>
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<tr>
<td>2 b 2..1'</td>
<td>[0,0,0]</td>
<td>x,1/2,0</td>
<td></td>
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<tr>
<td>2 a 2..1'</td>
<td>[0,0,0]</td>
<td>x,0,0</td>
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</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm1'  
  \(a^* = a \quad b^* = b\)
- Along [1,0,0] p2mg1'  
  \(a^* = -c \quad b^* = b\)
- Along [0,1,0] p2mg1'  
  \(a^* = c \quad b^* = a\)

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,1/4
Origin at $2'12_1$

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations:

1. $1$
2. $2 (0,0,1/2) \quad 0,0,z$
3. $2' \quad 0,y,1/4$
4. $2' \quad x,0,0$

1. $2 (0,0,0) \quad 0,0,0$
2. $2 (0,0,1/2) \quad 0,0,1/2$
3. $2' \quad 0,0,1/2'$
4. $2' \quad 0,0,0'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{array}{cccc}
4 & e & 1 & (1) x,y,z [u,v,w] \\
2 & d & .2' & 1/2,y,1/4 [u,0,w] \\
2 & c & .2' & 0,y,1/4 [u,0,w] \\
2 & b & 2'.. & x,1/2,0 [0,v,w] \\
2 & a & 2'.. & x,0,0 [0,v,w] \\
\end{array}
\]

Symmetry of Special Projections

Along [0,0,1] p2mm       Along [1,0,0] p2'mg'       Along [0,1,0] p2'mg'
\[a^* = a \quad b^* = b\] \[a^* = -c \quad b^* = b\] \[a^* = c \quad b^* = a\]
Origin at 0,0,z           Origin at x,0,0           Origin at 0,y,1/4
P22'2₁' 17.4.109

22'2' P22'2₁'

Orthorhombic

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations:

1. 1
   (1) 0,0,0
   (2) 0,0,1/2
   (3) 0,x,0
   (4) 0,y,0

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Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>2 d .2'</td>
<td>1/2,y,1/4 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 c .2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 2..</td>
<td>x,1/2,0 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2..</td>
<td>x,0,0 [u,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p'2'm'm'  Along [1,0,0]  p'2mg  Along [0,1,0]  p'2'm'g
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \quad \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \quad \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a} \)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,1/4
Origin at 212,

Asymmetric unit $0 \leq x < 1/2; \ 0 \leq y < 1/2; \ 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

1. $I$  
   (1) $0,0,0$
   (2) $0,0,1/2$
   (3) $0,y,1/4$
   (4) $x,0,0$

For $(1,0,0)$' + set

1. $t'$ $(1,0,0)$
   (1) $1,0,0$
   (2) $0,0,1/2$
   (3) $1/2,y,1/4$
   (4) $1,0,0$

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Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(0,0,0) + (1,0,0) +</td>
</tr>
<tr>
<td>4 d .2'</td>
<td>1/2,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 c .2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 b 2..</td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 a 2..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a.2m’m’          Along [1,0,0] p2mg1’          Along [0,1,0] p2b.2m’g’
\( \mathbf{a}^* = \mathbf{a} \) \hspace{1cm} \( \mathbf{b}^* = \mathbf{b} \) \hspace{1cm} \( \mathbf{a}^* = \mathbf{c} \) \hspace{1cm} \( \mathbf{b}^* = \mathbf{a} \)
Origin at 0,0,z                        Origin at x,0,0                        Origin at 0,y,1/4
**Symmetry Operations**

For \((0,0,0) +\) set

1. \((1)\, 1\)
2. \((2)\, (0,0,1/2)\, 0,0,z\)
3. \((3)\, 2\, 0,y,1/4\)
4. \((4)\, 2\, x,0,0\)

For \((1,0,0)'+\) set

1. \((1)\, t'\, (1,0,0)\)
2. \((2)\, 2'\, (0,0,1/2)\, 1/2,0,z\)
3. \((3)\, 2'\, 1/2,y,1/4\)
4. \((4)\, 2'\, (1,0,0)\, x,0,0\)

**Asymmetric unit**

\(0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) ( \bar{x}, \bar{y}, \bar{z} + 1/2 ) [( \bar{u}, \bar{v}, \bar{w} )]</td>
</tr>
<tr>
<td></td>
<td>(3) ( \bar{x}, \bar{y}, \bar{z} + 1/2 ) [( \bar{u}, \bar{v}, \bar{w} )]</td>
</tr>
<tr>
<td></td>
<td>(4) ( \bar{x}, \bar{y}, \bar{z} ) [( u, \bar{v}, \bar{w} )]</td>
</tr>
<tr>
<td>4 d .2'</td>
<td>1/2,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>4 c .2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,( \bar{y}, 3/4 ) [0,( \bar{v}, 0 )]</td>
</tr>
<tr>
<td>4 b 2'..</td>
<td>x,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>( \bar{x}, 1/2, 1/2 ) [0,( \bar{v}, \bar{w} )]</td>
</tr>
<tr>
<td>4 a 2'..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>( \bar{x}, 0, 1/2 ) [( u, 0, 0 )]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p_{c-2mm}</th>
<th>Along [1,0,0] p_{2mg1'}</th>
<th>Along [0,1,0] p_{2mg1'}</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) b^* = b \</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 1/2,1/2,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,1/4</td>
</tr>
</tbody>
</table>
Orthorhombic

$P_{2a} 2'2'2_1$

17.7.112

$2221'$

$P_{2a} 2'2'2_1$

**Origin** at $2'12_1$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

**Symmetry Operations**

For $(0,0,0)$ + set

1. $1$
   
   2. $2$ (0,0,1/2) 0,0,z
   
   3. $2'$ 0,y,1/4
   
   4. $2'$ 0,0,0

For $(1,0,0)'$ + set

1. $t'$ (1,0,0)
   
   2. $2'$ (0,0,1/2) 1/2,0,z
   
   3. $2$ 1/2,y,1/4
   
   4. $2$ (1,0,0) x,0,0
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>8</strong> e 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z+1/2 [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td><strong>4</strong> d .2</td>
<td>1/2,y,1/4 [0,v,0] 1/2,y,3/4 [0,v,0]</td>
</tr>
<tr>
<td><strong>4</strong> c .2'</td>
<td>0,y,1/4 [u,0,w] 0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td><strong>4</strong> b 2</td>
<td>x,1/2,0 [u,0,0] x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td><strong>4</strong> a 2</td>
<td>x,0,0 [u,0,0] x,0,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{2a}.2mm \) \( a^* = a \) \( b^* = b \) Origin at 0,0,z

Along [1,0,0] \( p2mg1' \) \( a^* = -c \) \( b^* = b \) Origin at x,0,0

Along [0,1,0] \( p_{2b}.2mg \) \( a^* = c \) \( b^* = a \) Origin at 1/2,y,1/4
Origin at intersection of 2 with perpendicular plane containing 2, axes

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) $1$
(2) $2 \ 0,0,z$
(3) $2 \ (0,1/2,0) \ 1/4,y,0$
(4) $2 \ (1/2,0,0) \ x,1/4,0$

(1) $0,0,0$
(2) $z,0,0,0$
(3) $y,1/2,1/2,0$
(4) $x,1/2,1/2,0$
Generators selected
(1); \(t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).\)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) (x,y,z [u,v,w]) (2) (\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]) (3) (x+1/2,y+1/2,z [u,v,w]) (4) (x+1/2,y+1/2,z [u,v,w])</td>
</tr>
<tr>
<td>2 b .2</td>
<td>(0,1/2,z [0,0,w]) (1/2,0,z [0,0,\bar{w}])</td>
</tr>
<tr>
<td>2 a .2</td>
<td>(0,0,z [0,0,w]) (1/2,1/2,z [0,0,\bar{w}])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2g'g' Along [1,0,0] p2m'g' Along [0,1,0] p2m'g'
\(a^* = a \quad b^* = b\) \(a^* = b \quad b^* = c\) \(a^* = -a \quad b^* = c\)
Origin at 0,0,z Origin at x,1/4,0 Origin at 1/4,y,0
Origin: at intersection of 21' with perpendicular plane containing 2,1' axes

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

**For 1 + set**

1. $1 \rightarrow 0,0,z$
2. $2 \rightarrow 0,0,0$
3. $2 \rightarrow (0,1/2,0) \rightarrow 1/4,y,0$
4. $2 \rightarrow (1/2,0,0) \rightarrow x,1/4,0$

**For 1' + set**

1. $1' \rightarrow 0,0,0'$
2. $2' \rightarrow 0,0,z$
3. $2' \rightarrow (0,1/2,0) \rightarrow 1/4,y,0$
4. $2' \rightarrow (1/2,0,0) \rightarrow x,1/4,0$

Orthorhombic

P2₂₂₁' 18.2.114

P2₂₂₁' 222₁'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3), 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>1 +</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 11'</td>
<td>x,y,z [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b ..21'</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a ..21'</td>
<td>0,0,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg1'  Along [1,0,0] p2mg1'  Along [0,1,0] p2mg1'

\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \quad \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \quad \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c} \)

Origin at 0,0,z

Origin at x,1/4,0

Origin at 1/4,y,0
Origin at intersection of 2 with perpendicular plane containing 2', axes

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) 1
   (0,0,0)

(2) 2 0,0,z
   (0,0,0)

(3) 2' (0,1/2,0) 1/4,1/2,0
   (0,1/2,0)

(4) 2' (1/2,0,0) x,1/2,0
   (1/2,0,0)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y, z [u, v, w]</td>
<td>(3) x+1/2, y+1/2, z [u, v, w]</td>
</tr>
<tr>
<td>2 b</td>
<td>0,1/2, z [0,0,w]</td>
<td>1/2,0, z [0,0,w]</td>
<td>1/2,1/2, z [0,0,w]</td>
</tr>
<tr>
<td>2 a</td>
<td>0,0, z [0,0,w]</td>
<td>1/2,1/2, z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg Along [1,0,0] p2'm'g Along [0,1,0] p2'm'g
a* = a b* = b a* = b b* = c a* = -a b* = c
Origin at 0,0,z Origin at x,1/4,0 Origin at 1/4,y,0
Origin: at intersection of 2' with perpendicular plane containing 2, and 2', axes

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations:

1. 1
2. 2', 0,0,z
3. 2' (0,1/2,0) 1/4,y,0
4. 2 (1/2,0,0) x,1/4,0
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 b ..2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>2 a ..2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(3) x+1/2,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2'gg'  
Along [1,0,0]  p2mg  
Along [0,1,0]  p2'mg'  

a* = a  b* = b  
a* = b  b* = c  
a* = -a  b* = c  

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at 1/4,y,0

18.4.116 - 2 - 209
Ortinhombic

Origin: at intersection of 2 with perpendicular plane containing 21 axes

Asymmetric unit:

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set:

1. $1$
2. $2, 0,0,z$
3. $2 (0,1/2,0) 1/4,y,0$
4. $2 (1/2,0,0) x,1/4,0$

For $(0,0,1)' +$ set:

1. $t (0,0,1)$
2. $2' (0,0,1) 0,0,z$
3. $2' (0,1/2,0) 1/4,y,1/2$
4. $2' (1/2,0,0) x,1/4,1/2$

For $(0,0,1)' -$ set:

1. $t (0,0,1)$
2. $2' (0,0,1) 0,0,z$
3. $2' (0,1/2,0) 1/4,y,1/2$
4. $2' (1/2,0,0) x,1/4,1/2$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1'); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 (b)</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 (a)</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2gg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2b2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,1/4,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p2b2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 1/4,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Orthorhombic

Origin at intersection of 2' with perpendicular plane containing 2, and 2', axes

Asymmetric unit

\[ 0 \leq x < \frac{1}{2}; \quad 0 \leq y < \frac{1}{2}; \quad 0 \leq z < 1 \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2', 0,0,z \\
(3) & \quad 2' (0,1/2,0) \quad 1/4,y,0 \\
(4) & \quad 2 (1/2,0,0) \quad x,1/4,0
\end{align*}
\]

For \((0,0,1)'+ \text{set}\)

\[
\begin{align*}
(1) & \quad t' (0,0,1) \\
(2) & \quad 2 (0,0,1) \quad 0,0,z \\
(3) & \quad 2 (0,1/2,0) \quad 1/4,y,1/2 \\
(4) & \quad 2' (1/2,0,0) \quad x,1/4,1/2
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(0,0,0) + (0,0,1) +</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>0,1/2,z [u,v,0] 1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>0,0,z [u,v,0] 1/2,1/2,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2gg1'</th>
<th>Along [1,0,0] p2b*2mg</th>
<th>Along [0,1,0] p2b*2mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a   b* = b</td>
<td>a* = b   b* = c</td>
<td>a* = -a  b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 1/4,y,1/2</td>
</tr>
</tbody>
</table>
Origin at midpoint of three non-intersecting pairs of parallel 2, axes

Asymmetric unit  
\[ 0 \leq x < \frac{1}{2}; \quad 0 \leq y < \frac{1}{2}; \quad 0 \leq z < 1 \]

Symmetry Operations

\begin{align*}
(1) & \quad \textbf{1} \\
(1') & \quad (0,0,0) \\
(2) & \quad 2 \cdot (0,0,1/2) \cdot 1/4,0,z \\
(2_z) & \quad 1/2,0,1/2 \\
(3) & \quad 2 \cdot (0,1/2,0) \cdot 0,y,1/4 \\
(2_y) & \quad 0,1/2,1/2 \\
(4) & \quad 2 \cdot (1/2,0,0) \cdot x,1/4,0 \\
(2_x) & \quad 1/2,1/2,0
\end{align*}
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 a 1</td>
<td>(1) x,y,z [u,v,w]  (2) x+1/2,y,z+1/2 [u,v,w] (3) x,y+1/2,z+1/2 [u,v,w] (4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2g'g'     Along [1,0,0] p2g'g'     Along [0,1,0] p2g'g'
\( a^* = a \) \( b^* = b \) \( c^* = c \) \( a^* = b \) \( b^* = c \) \( a^* = c \) \( b^* = a \)
Origin at 1/4,0,z        Origin at x,1/4,0        Origin at y,1/4,0
Origin at midpoint of three non-intersecting pairs of parallel \( 2_1' \) axes

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \( 1 \) + set

(1) \( 1 \)  
(1 | 0,0,0)

(2) \( 2 \) (0,0,1/2) 1/4,0,z  
(2 | 1/2,0,1/2)

(3) \( 2 \) (0,1/2,0) 0,y,1/4  
(2 | 0,1/2,1/2)

(4) \( 2 \) (1/2,0,0) x,1/4,0  
(2 | 1/2,1/2,0)

For \( 1' \) + set

(1) \( 1' \)  
(1 | 0,0,0')

(2) \( 2' \) (0,0,1/2) 1/4,0,z  
(2 | 1/2,0,1/2)

(3) \( 2' \) (0,1/2,0) 0,y,1/4  
(2 | 0,1/2,1/2)

(4) \( 2' \) (1/2,0,0) x,1/4,0  
(2 | 1/2,1/2,0)
Continued

19.2.120

P2₁,2,2,1’

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1’.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1’ +</td>
<td></td>
</tr>
<tr>
<td>4 a 11’ (1) x,y,z [0,0,0] (2) x+1/2,y,z+1/2 [0,0,0] (3) x,y+1/2,z+1/2 [0,0,0] (4) x+1/2,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2gg1’</th>
<th>Along [1,0,0] p2gg1’</th>
<th>Along [0,1,0] p2gg1’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = c b* = a</td>
</tr>
<tr>
<td>Origin at 1/4,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,1/4</td>
</tr>
</tbody>
</table>
Origin at midpoint of three non-intersecting pairs of parallel 2, and 2,’ axes

Asymmetric unit \(0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1\)

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1 & \quad 0,0,0) \\
(2) & \quad 2 (0,0,1/2) 1/4,0,z \\
(2 & \quad z 1/2,0,1/2) \\
(3) & \quad 2' (0,1/2,0) 0,y,1/4 \\
(2' & \quad y 0,1/2,1/2)' \\
(4) & \quad 2' (1/2,0,0) x,1/4,0 \\
(2' & \quad x 1/2,1/2,0)' \\
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 a 1</td>
<td>(1) x,y,z [u,v,w] (2) x+1/2,y,z+1/2 [u,v,w] (3) x,y+1/2,z+1/2 [u,v,w] (4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p2gg

- $a^* = a$
- $b^* = b$
- Origin at 1/4,0,z

Along [1,0,0] p2'gg'

- $a^* = -c$
- $b^* = b$
- Origin at x,1/4,0

Along [0,1,0] p2'gg'

- $a^* = c$
- $b^* = a$
- Origin at 0,y,1/4
Origin at \(212,1\)

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0)\) + set

1. \((1,0,0,0)\)
2. \((0,0,1/2,0), 0,0,z\)
3. \((2,0,0,1/2)\)
4. \((2,0,0,0)\)

For \((1/2,1/2,0)\) + set

1. \((1/2,1/2,0)\)
2. \((0,0,1/2,0), 1/4,1/4,z\)
3. \((2,0,1/2,0), 1/4,0,1/4\)
4. \((2,1/2,0,0)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry. Coefficients, Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 b .2</td>
<td>0,y,1/4 [0,v,0]</td>
<td>0,y,3/4 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 a 2..</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2m'm' Along [1,0,0] p2m'g' Along [0,1,0] p2m'g'

a* = a  b* = b  a* = -c  b* = b/2  a* = c  b* = a/2

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,1/4
**Origin** at 212,1'

**Asymmetric unit**

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \( (1) \quad 1 \)
2. \( (2) \quad 2 (0,0,1/2) \quad 0,0,z \)
   \( (2_z) \quad 0,0,1/2 \)
3. \( (3) \quad 2 \quad 0,y,1/4 \)
   \( (2_y) \quad 0,0,1/2 \)
4. \( (4) \quad 2 \quad x,0,0 \)
   \( (2_x) \quad 0,0,0 \)

For \((1/2,1/2,0)\) + set

1. \( (1) \quad t \)
   \( (1) \quad 1/2,1/2,0 \)
2. \( (2) \quad 2 (0,0,1/2) \quad 1/4,1/4,z \)
   \( (2_z) \quad 1/2,1/2,1/2 \)
3. \( (3) \quad 2 (0,1/2,0) \quad 1/4,y,1/4 \)
   \( (2_y) \quad 1/2,1/2,1/2 \)
4. \( (4) \quad 2 \quad (1/2,0,0) \quad x,1/4,0 \)
   \( (2_x) \quad 1/2,1/2,0 \)

For \((0,0,0)'\) + set

1. \( (1) \quad 1' \)
   \( (1) \quad 0,0,0' \)
2. \( (2) \quad 2' (0,0,1/2) \quad 0,0,z \)
   \( (2_z') \quad 0,0,1/2' \)
3. \( (3) \quad 2' (0,1/2,0) \quad 0,y,1/4 \)
   \( (2_y') \quad 0,0,1/2' \)
4. \( (4) \quad 2' \quad x,0,0 \)
   \( (2_x') \quad 0,0,0' \)

For \((1/2,1/2,0)'\) + set

1. \( (1) \quad t' \)
   \( (1) \quad 1/2,1/2,0' \)
2. \( (2) \quad 2' (0,0,1/2) \quad 1/4,1/4,z \)
   \( (2_z') \quad 1/2,1/2,1/2' \)
3. \( (3) \quad 2' (0,1/2,0) \quad 1/4,y,1/4 \)
   \( (2_y') \quad 1/2,1/2,1/2' \)
4. \( (4) \quad 2' (1/2,0,0) \quad x,1/4,0 \)
   \( (2_x') \quad 1/2,1/2,0' \)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 b .2.1'</td>
<td>0,y,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2..1'</td>
<td>x,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c b* = b/2</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c b* = a/2</td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,1/4
Origin at $2'12_1$

Asymmetric unit $0 \leq x < 1/2$; $0 \leq y < 1/2$; $0 \leq z < 1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
2. $(2) (0,0,1/2)$ $0,0,z$
3. $(2') (0,0,1/2)'$
4. $(4) 2' x,0,0$

For $(1/2,1/2,0) +$ set

1. $t (1/2,1/2,0)$
2. $(2) (0,0,1/2) 1/4,1/4,z$
3. $(2') (0,1/2,0) 1/4,y,1/4$
4. $(4) 2' (1/2,0,0) x,1/4,0$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 a 2'..</td>
<td>x,0,0 [v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm</th>
<th>Along [1,0,0]</th>
<th>p2'mg'</th>
<th>Along [0,1,0]</th>
<th>p2'mg'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -c</td>
<td>b* = b/2</td>
<td>a* = c</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,1/4</td>
<td></td>
</tr>
</tbody>
</table>
Origin at 212, 1

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 (1 | 0,0,0)
(2) 2' (0,0,1/2) 0,0,z
(2 | 0,0,1/2)'
(3) 2' 0,y,1/4
(2 | 0,0,1/2)'
(4) 2 x,0,0
(2 | 0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1 | 0,0,0)
(2) 2' (0,0,1/2) 1/4,1/4,z
(2 | 1/2,1/2,1/2)'
(3) 2' (0,1/2,0) 1/4,y,1/4
(2 | 1/2,1/2,1/2)'
(4) 2 (1/2,0,0) x,1/4,0
(2 | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 a 2..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Axial Direction</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>c2'mm'</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2mg</td>
</tr>
<tr>
<td>Along [0,1,0]</td>
<td>p2m'g</td>
</tr>
</tbody>
</table>

**Generators**

- (1) = t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)
- (2) = t(1,0,0); t(0,1,0); t(0,0,1)
- (3) = t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)
Origin at 212,

Asymmetric unit: $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set:

1. $1$
2. $2 (0,0,1/2) 0,0,z$
3. $2 (0,1/2,0) 1/4,y,1/4$
4. $2 x,0,0$

For $(1/2,1/2,0)'$ + set:

1. $t' (1/2,1/2,0)$
2. $2' (0,0,1/2) 1/4,1/4,z$
3. $2' (0,1/2,0) 1/4,y,1/4$
4. $2' (1/2,0,0) x,1/4,0$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(0,0,0) + (1/2,1/2,0) ' +</td>
</tr>
<tr>
<td>4 b .2</td>
<td>0, y, 1/4 [0, v, 0]</td>
</tr>
<tr>
<td>4 a 2</td>
<td>x, 0, 0 [u, 0, 0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0, 0, 1] \( c_{p2m'm'} \)
  - \( a^* = a \) \( b^* = b \)
  - Origin at 0, 0, z

- Along [1, 0, 0] \( p_{2b'2m'g'} \)
  - \( a^* = -c \) \( b^* = b/2 \)
  - Origin at x, 0, 0

- Along [0, 1, 0] \( p_{2v'2m'g'} \)
  - \( a^* = c \) \( b^* = a/2 \)
  - Origin at y, 0, 1/4
Orthorhombic

CP$_2$'2'2$_1$

20.6.127

CP$_2$'2'2$_1$

Origin at 2'12$_1$

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2$_z$ | 0,0,1/2)

(3) 2' 0,y,1/4
(2$_y$ | 0,0,1/2$_1$)

(4) 2' x,0,0
(2$_x$ | 0,0,0$_1$)

For (1/2,1/2,0)$_1$ + set

(1) t' (1/2,1/2,0) 0,1/2,0
(1 | 1/2,1/2,0)$_1$

(2) 2' (0,0,1/2) 1/4,1/4,z
(2$_z$ | 1/2,1/2,1/2$_1$)

(3) 2 (0,1/2,0) 1/4,y,1/4
(2$_y$ | 1/2,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2$_x$ | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>8</th>
<th>c</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(0,0,0) + (1/2,1/2,0)' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>b</td>
<td>.2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>2'</td>
<td>x,0,0 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  \( \text{c}_{\text{p}} \text{2mm} \)  Along [1,0,0]  \( \text{p}_{\text{2b}} \text{2mg} \)  Along [0,1,0]  \( \text{p}_{\text{2b}} \text{2mg} \)  
\( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)  \( \mathbf{a}^* = -\mathbf{c} \)  \( \mathbf{b}^* = \mathbf{b}/2 \)  \( \mathbf{a}^* = \mathbf{c} \)  \( \mathbf{b}^* = \mathbf{a}/2 \)  
Origin at 0,0,z  Origin at x,1/4,0  Origin at 1/4,y,1/4
Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1 | 0,0,0)

(2) 2' (0,0,1/2) 0,0,z
    (2z | 0,0,1/2)'

(3) 2' 0,y,1/4
    (2y | 0,0,1/2)'

(4) 2 x,0,0
    (2x | 0,0,0)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
    (1 | 1/2,1/2,0)'

(2) 2 (0,0,1/2) 1/4,1/4,z
    (2y | 1/2,1/2,1/2)

(3) 2 (0,1/2,0) 1/4,y,1/4
    (2y | 1/2,1/2,1/2)

(4) 2' (1/2,0,0) x,1/4,0
    (2z | 1/2,1/2,0)'

Origin at 212,'
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z+1/2 [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>0,y,1/4 [u,0,w] 0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>4 a 2.</td>
<td>x,0,0 [u,0,0] x,0,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c_p2'2mm'</th>
<th>Along [1,0,0]</th>
<th>p_ab-2mg</th>
<th>Along [0,1,0]</th>
<th>p_2v-2mg'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -c</td>
<td>b* = b/2</td>
<td>a* = c</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 1/4,y,1/4</td>
<td></td>
</tr>
</tbody>
</table>
Orthorhombic

C222 21.1.129 C222

Origin at 222

Asymmetric unit

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 0,0,z \\
(3) & \quad 2 \quad 0,0,0 \\
(4) & \quad 2 \quad z,0,0
\end{align*}
\]

For \((1/2,1/2,0)\) + set

\[
\begin{align*}
(1) & \quad t \quad 1/2,1/2,0 \\
(2) & \quad 1/4,1/4,z \\
(3) & \quad 2 \quad 0,1/2,0 \\
(4) & \quad 2 \quad 1/2,0,0
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 8 | l | 1 | (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] |
| 4 | k | .2 | 1/4,1/4,z [0,0,w] | 3/4,1/4,z [0,0,w] |
| 4 | j | .2 | 0,1/2,z [0,0,w] | 0,1/2,z [0,0,w] |
| 4 | i | .2 | 0,0,z [0,0,w] | 0,0,z [0,0,w] |
| 4 | h | .2 | 0,y,1/2 [0,v,0] | 0,y,1/2 [0,v,0] |
| 4 | g | .2 | 0,y,0 [0,v,0] | 0,y,0 [0,v,0] |
| 4 | f | .2 | x,0,1/2 [u,0,0] | x,0,1/2 [u,0,0] |
| 4 | e | .2 | x,0,0 [u,0,0] | x,0,0 [u,0,0] |
| 2 | d | 222 | 0,0,1/2 [0,0,0] |
| 2 | c | 222 | 1/2,0,1/2 [0,0,0] |
| 2 | b | 222 | 0,1/2,0 [0,0,0] |
| 2 | a | 222 | 0,0,0 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1]  c2m'm'  Along [1,0,0]  p2m'm'  Along [0,1,0]  p2m'm'  
\( a^* = a \)  \( b^* = b \)  \( a^* = b/2 \)  \( b^* = c \)  \( a^* = c \)  \( b^* = a/2 \)  
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Asymmetric unit $0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

1. $1 \ (0,0,0)$
2. $2 \ 0,0,z \ (2z|0,0,0)$
3. $2 \ 0,y,0 \ (2y|0,0,0)$
4. $2 \ x,0,0 \ (2x|0,0,0)$

For $(1/2,1/2,0)$ + set

1. $t \ (1/2,1/2,0) \ (1/2,1/2,0)$
2. $2 \ 1/4,1/4,z \ (2z|1/2,1/2,0)$
3. $2 \ (0,1/2,0) \ 1/4,y,0 \ (2y|1/2,1/2,0)$
4. $2 \ (1/2,0,0) \ x,1/4,0 \ (2x|1/2,1/2,0)$

For $(0,0,0)'$ + set

1. $1' \ (0,0,0)'$
2. $2' \ 0,0,z \ (2z|0,0,0)'$
3. $2' \ 0,y,0 \ (2y|0,0,0)'$
4. $2' \ x,0,0 \ (2x|0,0,0)'$

For $(1/2,1/2,0)'$ + set

1. $t' \ (1/2,1/2,0)' \ (1/2,1/2,0)'$
2. $2' \ 1/4,1/4,z \ (2z|1/2,1/2,0)'$
3. $2' \ (0,1/2,0)' \ 1/4,y,0 \ (2y|1/2,1/2,0)'$
4. $2' \ (1/2,0,0)' \ x,1/4,0 \ (2x|1/2,1/2,0)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' +</td>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>8 l 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 k .21' 1/4,1/4,z [0,0,0] 3/4,1/4,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 j .21' 0,1/2,z [0,0,0] 0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 i .21' 0,0,z [0,0,0] 0,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 h .21' 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 g .21' 0,y,0 [0,0,0] 0,y,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 f .21' x,0,1/2 [0,0,0] x,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e .21' x,0,0 [0,0,0] x,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 d 2221' 0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 c 2221' 1/2,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b 2221' 0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2221' 0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

| Along [0,0,1] | c2mm1' | | Along [1,0,0] | p2mm1' | | Along [0,1,0] | p2mm1' |
|---------------|--------|---------------------------------|--------|---------------------------------|--------|
| a* = a b* = b | a* = b/2 b* = c | a* = c b* = a/2 |
| Origin at 0,0,z | Origin at x,0,0 | Origin at 0,y,0 |
C2'2'2 21.3.131

Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1) 0,0,0
(2) 2 0,0,z
   (2) 0,0,0
(3) 2' 0,y,0
   (3) 1/2,0,0
(4) 2' x,0,0
   (4) 1/2,0,0

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
   (1) 1/2,1/2,0
(2) 2 1/4,1/4,z
   (2) 1/2,1/2,0
(3) 2' (0,1/2,0) 1/4,y,0
   (3) 1/2,1/2,0
(4) 2' (1/2,0,0) x,1/4,0
   (4) 1/2,1/2,0

Origin at 2'2'2
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>8</td>
<td>l</td>
</tr>
<tr>
<td>4</td>
<td>k</td>
</tr>
<tr>
<td>4</td>
<td>j</td>
</tr>
<tr>
<td>4</td>
<td>i</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
</tr>
<tr>
<td>4</td>
<td>f</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm

\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)

Origin at 0,0,z

Along [1,0,0] p2'\text{mm}'

\( \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)

Origin at 0,0,0

Along [0,1,0] p2'\text{mm}'

\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}/2 \)

Origin at 0,y,0
Asymmetric unit: $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

**Symmetry Operations**

For $(0,0,0) +$ set:

1. $(2^* 0,0,0)$
2. $(2^* 0,0,0)'$
3. $(2^* 0,0,0)''$
4. $(2^* 0,0,0)'''$

For $(1/2,1/2,0) +$ set:

1. $(2^* 1/4,1/4,0)$
2. $(2^* 1/4,1/4,0)'$
3. $(2^* 1/4,1/4,0)''$
4. $(2^* 1/4,1/4,0)'''$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1 (1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 k .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>4 j .2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 i .2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 h .2'</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 g .2'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 f .2'</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 e .2'</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2 d 22'2'</td>
<td>0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 c 22'2'</td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 b 22'2'</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>2 a 22'2'</td>
<td>0,0,0 [u,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] c'2mm'
- Along [1,0,0] p2mm
- Along [0,1,0] p2'2mm'

\[
\begin{align*}
\mathbf{a^*} &= \mathbf{a} & \mathbf{b^*} &= \mathbf{b} \\
\mathbf{a^*} &= \mathbf{b}/2 & \mathbf{b^*} &= \mathbf{c} \\
\mathbf{a^*} &= -\mathbf{a}/2 & \mathbf{b^*} &= \mathbf{c} \\
\text{Origin at 0,0,z} & & \text{Origin at x,0,0} & & \text{Origin at 0,y,0}
\end{align*}
\]
**Asymmetric unit**

\[ 0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \((1)\) 1
2. \((2)\) 2, \(0,0,z\)
3. \((3)\) 2, \(0,y,0\)
4. \((4)\) 2, \(x,0,0\)

For \((1/2,1/2,0) + \) set

1. \((1)\) 1, \(1/2,1/2,0\)
2. \((2)\) 2, \(1/4,1/4,z\)
3. \((3)\) 2, \(0,1/2,0\)
4. \((4)\) 2, \(1/2,0,0\)

For \((0,0,1) + \) set

1. \((1)\) 1, \(0,0,1\)
2. \((2)\) 2, \(0,0,1\), \(0,0,z\)
3. \((3)\) 2, \(0,1/2,0\)
4. \((4)\) 2, \(1/2,0,0\)

For \((1/2,1/2,1) + \) set

1. \((1)\) 1, \(1/2,1/2,1\)
2. \((2)\) 2, \(0,0,1\), \(1/4,1/4,z\)
3. \((3)\) 2, \(0,1/2,0\)
4. \((4)\) 2, \(1/2,0,0\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 l</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 k</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 j</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 i</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>8 f</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>0,0,1/2 [0,w]</td>
</tr>
<tr>
<td>4 c</td>
<td>1/2,0,1/2 [0,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,0,0] p2mm' Along [0,1,0] p2mm'  
\(a^* = a\) \(b^* = b\)  
\(a^* = -c\) \(b^* = b/2\)  
\(a^* = c\) \(b^* = a/2\)  
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1|0,0,0)

(2) 2  0,0,z
    (2z|0,0,0)

(3) 2  0,y,0
    (2y|0,0,0)

(4) 2  x,0,0
    (2x|0,0,0)

For (1/2,1/2,0)' + set

(1) 1' (1/2,1/2,0)
    (1|1/2,1/2,0)

(2) 2' 1/4,1/4,z
    (2z|1/2,1/2,0)

(3) 2' (0,1/2,0) 1/4,y,0
    (2y|1/2,1/2,0)

(4) 2' (1/2,0,0) x,1/4,0
    (2x|1/2,1/2,0)
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'\); \((2); (3)\).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0) + (1/2,1/2,0)' +)</td>
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<table>
<thead>
<tr>
<th>8 l 1</th>
<th>((1) \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}])</th>
<th>((2) \bar{x}, \bar{y}, \bar{z} [u, v, w])</th>
<th>((3) \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}])</th>
<th>((4) x, y, z [u, v, w])</th>
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<tbody>
<tr>
<td>4 k 2'</td>
<td>((1/2,1/2,0))</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>4 j 2</td>
<td>((0,1/2,0))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 i 2</td>
<td>((0,0,0))</td>
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<td>4 h 2</td>
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<tr>
<td>4 g 2</td>
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<tr>
<td>4 f 2</td>
<td>((0,0,0))</td>
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<td></td>
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</tr>
<tr>
<td>4 e 2</td>
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<tr>
<td>2 d 222</td>
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<td></td>
</tr>
<tr>
<td>2 c 222</td>
<td>((1/2,0,1/2))</td>
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<td></td>
</tr>
<tr>
<td>2 b 222</td>
<td>((0,1/2,0))</td>
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<td></td>
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</tr>
<tr>
<td>2 a 222</td>
<td>((0,0,0))</td>
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<td></td>
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</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \(c_{p}2m'm'\)
- Along \([1,0,0]\) \(p_{2a}2m'm'\)
- Along \([0,1,0]\) \(p_{2a}2m'm'\)

\(a^* = a, b^* = b\)  
Origin at \(0,0,z\)

\(a^* = b/2, b^* = c\)  
Origin at \(x,0,0\)

\(a^* = -a/2, b^* = c\)  
Origin at \(0,y,0\)
Asymmetric unit: $0 < x < 1/4; \ 0 < y < 1/2; \ 0 < z < 1$

### Symmetry Operations

**For (0,0,0) + set**

1. $t \ (0,0,0) \\
   (1 \ 0,0,0)
2. $2 \ 0,0,z$ \\
   $(2z \ 0,0,0)$
3. $2 \ 0,y,0$ \\
   $(2y \ 0,0,0)$
4. $2 \ x,0,0$ \\
   $(2x \ 0,0,0)$

**For (1/2,1/2,0) + set**

1. $t' \ (1/2,1/2,0) \\
   (1 \ 1/2,1/2,0)$
2. $2' \ 1/4,1/4,z$ \\
   $(2z' \ 1/2,1/2,0)$
3. $2' \ (0,1/2,0)$ \\
   $(2y' \ 1/2,1/2,0)$
4. $2' \ (1/2,0,0)$ \\
   $(2x' \ 1/2,1/2,0)$

**For (0,0,1) + set**

1. $t' \ (0,0,1) \\
   (1 \ 0,0,1)$
2. $2' \ (0,0,1)$ \\
   $(2z' \ 0,0,1)$
3. $2' \ 0,y,1/2$ \\
   $(2y' \ 0,0,1)$
4. $2' \ x,0,1/2$ \\
   $(2x' \ 0,0,1)$

**For (1/2,1/2,1) + set**

1. $t \ (1/2,1/2,1) \\
   (1 \ 1/2,1/2,1)$
2. $2 \ (0,0,1)$ \\
   $(2z \ 1/2,1/2,1)$
3. $2 \ (0,1/2,0)$ \\
   $(2y \ 1/2,1/2,1)$
4. $2 \ (1/2,0,0)$ \\
   $(2x \ 1/2,1/2,1)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(0,0,1) + (1/2,1/2,1)</td>
<td></td>
</tr>
<tr>
<td>(0,0,0) + (1/2,1/2,0)’</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(0,0,1)’ + (1/2,1/2,1)’</td>
<td></td>
</tr>
</tbody>
</table>

| 16 l 1 | (1) x,y,z [u,v,w] |
| 8 k .2’ | 1/4,1/4,z [u,v,0] |
| 8 j .2 | 0,1/2,z [0,0,w] |
| 8 i .2 | 0,0,z [0,0,w] |
| 8 h .2’ | 0,y,1/2 [u,0,w] |
| 8 g .2 | 0,y,0 [v,0] |
| 8 f .2’ | x,0,1/2 [0,v,w] |
| 8 e .2 | x,0,0 [u,0,0] |
| 4 d .2’2 | 0,0,1/2 [0,0,w] |
| 4 c .2’2 | 1/2,0,1/2 [0,0,w] |
| 4 b .2’2 | 0,1/2,0 [0,0,0] |
| 4 a .2’2 | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b/2 b* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at x,1/4,1/2</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c b* = a/2</td>
<td></td>
</tr>
<tr>
<td>Origin at 1/4,y,1/2</td>
<td></td>
</tr>
</tbody>
</table>

21.7.135 - 2 - 247
Asymmetric unit: $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

(1) $1$ 
(2) $2' \quad 0,0,z$ 
(3) $2' \quad 0,y,0$ 
(4) $2 \quad x,0,0$

For $(1/2,1/2,0) +$ set

(1) $t \quad (1/2,1/2,0)$ 
(2) $2' \quad 1/4,1/4,z$ 
(3) $2' \quad (0,1/2,0)$ 
(4) $2 \quad (1/2,0,0)$

For $(0,0,1)' +$ set

(1) $t' \quad (0,0,1)$ 
(2) $2 \quad (0,0,1) \quad 0,0,z$ 
(3) $2 \quad 0,y,1/2$ 
(4) $2' \quad x,0,1/2$

For $(1/2,1/2,1)' +$ set

(1) $t' \quad (1/2,1/2,1)$ 
(2) $2 \quad (0,0,1) \quad 1/4,1/4,z$ 
(3) $2 \quad (0,1/2,0) \quad 1/4,y,1/2$ 
(4) $2' \quad (1/2,0,0) \quad x,1/4,1/2$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>(0,0,1') +</td>
<td>(1/2,1/2,1') +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16 l 1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) (x',y',z [u,v,w])</th>
<th>(3) (x,y,\bar{z} [u,v,w])</th>
<th>(4) (x',y',\bar{z} [u,v,w])</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 k .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
<td>3/4,1/4,(\bar{z}) [u,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 j .2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>0,1/2,(\bar{z}) [u,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 i .2'</td>
<td>0,0,z [u,v,0]</td>
<td>0,0,(\bar{z}) [u,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 h .2'</td>
<td>0,y,1/2 [0,v,0]</td>
<td>0,(\bar{y}),1/2 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 g .2'</td>
<td>0,y,0 [u,0,w]</td>
<td>0,(\bar{y}),0 [u,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 f .2'</td>
<td>x,0,1/2 [0,v,w]</td>
<td>(\bar{x},0,1/2 [0,v,w])</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 e .2'</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 d 2'2'</td>
<td>0,0,1/2 [0,v,o]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 c 2'2'</td>
<td>1/2,0,1/2 [0,v,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 b 2'2'</td>
<td>0,1/2,0 [u,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 a 2'2'</td>
<td>0,0,0 [u,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a) (b^* = b)</td>
<td>(a^* = a) (b^* = b/2)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>(p_{2\alpha},2mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = -c) (b^* = b/2)</td>
<td>(a^* = c) (b^* = a/2)</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td>Origin at 1/4,y,0</td>
</tr>
</tbody>
</table>
CP2'2'2
21.9.137
C_{p2'2'2}'

Orthorhombic

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z
(3) 2' 0,y,0
(4) 2' x,0,0
(1*) 0,0,0
(2*) 0,0,0
(2y*) 0,0,0
(2x*) 0,0,0

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(2) 2' 1/4,1/4,z
(3) 2 (0,1/2,0) 1/4,y,0
(4) 2 (1/2,0,0) x,1/4,0
(1*) 1/2,1/2,0
(2*) 1/2,1/2,0
(2y*) 1/2,1/2,0
(2x*) 1/2,1/2,0
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>8 l 1 (1) x,y,z [u,v,w]</td>
<td>(2) $\bar{x},y,z [u\bar{v},w]$</td>
</tr>
<tr>
<td>4 k .2' 1/4,1/4,z [u,v,0]</td>
<td>3/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>4 j .2 0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 i .2 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 h .2' 0,y,1/2 [u,0,w]</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 g .2' 0,y,0 [u,0,w]</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 f .2' x,0,1/2 [0,v,w]</td>
<td>$\bar{x},0,1/2 [0,v,w]$</td>
</tr>
<tr>
<td>4 e .2' x,0,0 [0,v,w]</td>
<td>$\bar{x},0,0 [0,v,w]$</td>
</tr>
<tr>
<td>2 d 2'2' 0,0,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 c 2'2' 1/2,0,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 2'2' 0,1/2,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 a 2'2' 0,0,0 [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c$_p$2mm</th>
<th>Along [1,0,0]</th>
<th>p$_{2a}$2mm</th>
<th>Along [0,1,0]</th>
<th>p$_{2a}$2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a$^*$ = a</td>
<td>b$^*$ = b</td>
<td>a$^*$ = b/2</td>
<td>b$^*$ = c</td>
<td>a$^*$ = -a/2</td>
<td>b$^*$ = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,1/4</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Orthorhombic

Asymmetric unit

0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) 1

(1) t' (1/2,1/2,0)

(2) 2' 0,0,z

(2) 2 1/4,1/4,z

(2) 2 (0,1/2,0) 1/4,y,0

(2) 2' (1/2,0,0) x,1/4,0

(2) |0,0,0)

(2 |0,0,0)'

(2 z |0,0,0)'

(2 y |0,0,0)'

(2 x |0,0,0)'

For (1/2,1/2,0)' + set

(1) 1

(1) t' (1/2,1/2,0)

(2) 2 1/4,1/4,z

(2) 2 (0,1/2,0) 1/4,y,0

(2) 2' (1/2,0,0) x,1/4,0
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>I 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>k ..2</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>j ..2'</td>
<td>0,1/2,0 [u,v,0]</td>
<td>0,1/2,0 [u,v,0]</td>
</tr>
<tr>
<td>4</td>
<td>i ..2'</td>
<td>0,0,0 [u,v,0]</td>
<td>0,0,0 [u,v,0]</td>
</tr>
<tr>
<td>4</td>
<td>h ..2'</td>
<td>0,0,0 [u,v,0]</td>
<td>0,0,0 [u,v,0]</td>
</tr>
<tr>
<td>4</td>
<td>g ..2'</td>
<td>x,0,1/2 [u,v,0]</td>
<td>x,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4</td>
<td>e ..2'</td>
<td>x,0,0 [u,v,0]</td>
<td>x,0,0 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>d 22'2'</td>
<td>0,0,1/2 [u,v,0]</td>
<td>0,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>c 22'2'</td>
<td>1/2,0,1/2 [u,v,0]</td>
<td>1/2,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>b 22'2'</td>
<td>0,1/2,0 [u,v,0]</td>
<td>0,1/2,0 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 22'2'</td>
<td>0,0,0 [u,v,0]</td>
<td>0,0,0 [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_{p2}2'2'm'  Along [1,0,0] p_{2a}22'mm  Along [0,1,0] p_{2a}22'm'm'

*a* = a  b* = b  
Origin at 0,0,z  
Origin at x,0,0  
Origin at 1/4,y,0
CI 2'22' 2221' Orthorhombic

Origin at 2'22'

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

1. \((1,0,0,0)\)
2. \(2'0,0,z\)
3. \(20,y,0\)
4. \(2'x,0,0\)

For \((1/2,1/2,0)\)' + set

1. \((1/2,1/2,0)\)'
2. \(21/4,1/4,z\)
3. \(2'0,1/2,0\)
4. \(2x,1/4,0\)

For \((0,0,1)\)' + set

1. \((0,0,1)\)'
2. \(2(0,0,1)\)
3. \(2'0,y,1/2\)
4. \(2x,0,1/2\)

For \((1/2,1/2,1)\) + set

1. \((1/2,1/2,1)\)
2. \(2'(0,0,1)\) 1/4,1/4,z
3. \(2(0,1/2,0)\) 1/4,y,1/2
4. \(2'(1/2,0,0)\) x,1/4,1/2
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 k</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 j</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>8 f</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 e</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>4 d</td>
<td>0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,v,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**
  - c2mm1’

- **Along [1,0,0]**
  - p,2mm

- **Along [0,1,0]**
  - p,2mm

- **Origin at 0,0,z**

- **Origin at x,0,1/2**

- **Origin at 1/4,y,1/2**
**Symmetry Operations**

### For (0,0,0) + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(2) 2 0,0,z</td>
<td>(3) 2 0,y,0</td>
<td>(4) 2 x,0,0</td>
</tr>
<tr>
<td>(1</td>
<td>0,0,0)</td>
<td>(2</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

### For (0,1/2,1/2) + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (0,1/2,1/2)</td>
<td>(2) 2 (0,0,1/2) 0,1/4,z</td>
<td>(3) 2 (0,1/2,0) 0,y,1/4</td>
<td>(4) 2 x,1/4,1/4</td>
</tr>
<tr>
<td>(1</td>
<td>0,1/2,1/2)</td>
<td>(2</td>
<td>1/2,1/2)</td>
</tr>
</tbody>
</table>

### For (1/2,0,1/2) + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (1/2,0,1/2)</td>
<td>(2) 2 (0,0,1/2) 1/4,0,z</td>
<td>(3) 2 1/4,y,1/4</td>
<td>(4) 2 (1/2,0,0) x,0,1/4</td>
</tr>
<tr>
<td>(1</td>
<td>1/2,0,1/2)</td>
<td>(2</td>
<td>1/2,1/2)</td>
</tr>
</tbody>
</table>

### For (1/2,1/2,0) + set

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (1/2,1/2,0)</td>
<td>(2) 2 1/4,1/4,z</td>
<td>(3) 2 (0,1/2,0) 1/4,y,0</td>
<td>(4) 2 (1/2,0,0) x,1/4,0</td>
</tr>
<tr>
<td>(1</td>
<td>1/2,1/2,0)</td>
<td>(2</td>
<td>1/2,1/2)</td>
</tr>
</tbody>
</table>
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>16 k 1 (1) x,y,z [u,v,w]</td>
<td>(2) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
</tr>
<tr>
<td>8 j 2. x,1/4,1/4 [u,0,0]</td>
<td>3/4 x̅,1/4 [u̅,0,0]</td>
</tr>
<tr>
<td>8 i .2 1/4,y,1/4 [0,v,0]</td>
<td>3/4 y̅,1/4 [0̅,v̅,0]</td>
</tr>
<tr>
<td>8 h .2 1/4,1/4,z [0,0,w]</td>
<td>3/4,1/4,z̅ [0̅,0̅,w̅]</td>
</tr>
<tr>
<td>8 g .2 0,0,z [0,0,w]</td>
<td>0,0,z̅ [0̅,0̅,w̅]</td>
</tr>
<tr>
<td>8 f .2 0,y,0 [0,v,0]</td>
<td>0̅,y̅,0 [0̅,v̅,0]</td>
</tr>
<tr>
<td>8 e 2. x,0,0 [u,0,0]</td>
<td>x̅,0,0 [u̅,0,0]</td>
</tr>
<tr>
<td>4 d 222 1/4,1/4,3/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 c 222 1/4,1/4,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b 222 0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a 222 0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p2m' \( \mathbf{a}^* = \mathbf{a}/2 \) \( \mathbf{b}^* = \mathbf{b}/2 \)  
Origin at \( 0,0,z \)  
Along [1,0,0] p2m' \( \mathbf{a}^* = \mathbf{b}/2 \) \( \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at \( x,0,0 \)  
Along [0,1,0] p2m' \( \mathbf{a}^* = \mathbf{c}/2 \) \( \mathbf{b}^* = \mathbf{a}/2 \)  
Origin at \( 0,y,0 \)
Asymmetric unit: \[0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1\]

Symmetry Operations:

For \((0,0,0)\) + set:

1. \(1\) \((0,0,0)\)
2. \(2\) \((0,0,z)\)
3. \(3\) \((0,y,0)\)
4. \(4\) \((x,0,0)\)

For \((0,1/2,1/2)\) + set:

1. \(t\) \((0,1/2,1/2)\)
2. \(2\) \((0,0,1/2)\)
3. \(3\) \((1/2,0,1/2)\)
4. \(4\) \((1/2,0,0)\)

For \((1/2,0,1/2)\) + set:

1. \(t\) \((1/2,0,1/2)\)
2. \(2\) \((1/4,1/2,0)\)
3. \(3\) \((1/2,1/4,y)\)
4. \(4\) \((x,1/4,0)\)

For \((0,0,0)'\) + set:

1. \(1'\) \((0,0,0)\)
2. \(2'\) \((0,0,0)'\)
3. \(3'\) \((0,y,0)'\)
4. \(4'\) \((x,0,0)'\)

For \((0,1/2,1/2)'\) + set:

1. \(t'\) \((0,1/2,1/2)\)
2. \(2'\) \((0,0,1/2)\)
3. \(3'\) \((1/2,0,1/2)\)
4. \(4'\) \((x,1/4,0)\)
Continued

For \((1/2,0,1/2)' +\) set

\begin{align*}
(1) \ t' (1/2,0,1/2) \\
(1/2,0,1/2)' \quad (2) \ 2' (0,0,1/2) & \ 1/4,0,z \\
(2_2|1/2,0,1/2)' \quad (3) \ 2' 1/4,y,1/4 & \ 1/4,y,0 \\
& \ (2_2|1/2,0,1/2)' \quad (4) \ 2' (1/2,0,0) & \ x,0,1/4 \\
& \ (2_2|1/2,0,1/2)' \quad (2_2|1/2,0,1/2)'
\end{align*}

For \((1/2,1/2,0)' +\) set

\begin{align*}
(1) \ t' (1/2,1/2,0) \\
(1/2,1/2,0)' \quad (2) \ 2' 1/4,1/4,z & \ 1/4,1/4,z \\
(2_2|1/2,1/2,0)' \quad (3) \ 2' (0,1/2,0) & \ 1/4,y,0 \\
& \ (2_2|1/2,1/2,0)' \quad (4) \ 2' (1/2,0,0) & \ x,1/4,0 \\
& \ (2_2|1/2,1/2,0)' \quad (2_2|1/2,1/2,0)'
\end{align*}

Generators selected \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); 1'\).

Positions

\begin{align*}
\text{Multiplicity,} & \quad \text{Coordinates} \\
\text{Wyckoff letter,} & \quad (0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + \\
\text{Site Symmetry.} & \quad (0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)'
\end{align*}

\begin{align*}
& 16 \ k \ 11' \quad (1) \ x,y,z \ [0,0,0] \\
& 8 \ j \ 2.1' \quad x,1/4,1/4 \ [0,0,0] \\
& 8 \ i \ .2.1' \quad 1/4,y,1/4 \ [0,0,0] \\
& 8 \ h \ .21' \quad 1/4,1/4,z \ [0,0,0] \\
& 8 \ g \ .21' \quad 0,0,z \ [0,0,0] \\
& 8 \ f \ .2.1' \quad 0,y,0 \ [0,0,0] \\
& 8 \ e \ 2..1' \quad x,0,0 \ [0,0,0] \\
& 4 \ d \ 2221' \quad 1/4,1/4,3/4 \ [0,0,0] \\
& 4 \ c \ 2221' \quad 1/4,1/4,1/4 \ [0,0,0] \\
& 4 \ b \ 2221' \quad 0,0,1/2 \ [0,0,0] \\
& 4 \ a \ 2221' \quad 0,0,0 \ [0,0,0]
\end{align*}

Symmetry of Special Projections

Along \([0,0,1]\) p2mm1' \quad Along \([1,0,0]\) p2mm1' \quad Along \([0,1,0]\) p2mm1'
\begin{align*}
a^* & = a/2 \quad b^* = b/2 \\
a^* & = b/2 \quad b^* = c/2 \\
a^* & = c/2 \quad b^* = a/2 \\
\text{Origin at 0,0,z} & \quad \text{Origin at x,0,0} \\
\text{Origin at 0,y,0} &
\end{align*}
Origin at 2'2'2

Asymmetric unit

\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1\]

Symmetry Operations

For (0,0,0) + set

1. \(\mathbf{1}\)
2. \(\mathbf{2}\) \(0,0,z\)
3. \(\mathbf{2}'\) \(0,0,0\)^{'}
4. \(\mathbf{2}'\) \(x,0,0\)

For \((0,1/2,1/2) + set\)

1. \(\mathbf{1}\) \((0,1/2,1/2)\)
2. \(\mathbf{2}\) \(0,0,1/2\)
3. \(\mathbf{2}'\) \(0,1/2,0\)
4. \(\mathbf{2}'\) \(x,1/4,1/4\)

For \((1/2,0,1/2) + set\)

1. \(\mathbf{1}\) \((1/2,0,1/2)\)
2. \(\mathbf{2}\) \(1/4,0,z\)
3. \(\mathbf{2}'\) \(1/4,1/4,0\)
4. \(\mathbf{2}'\) \(x,0,1/4\)

For \((1/2,1/2,0) + set\)

1. \(\mathbf{1}\) \((1/2,1/2,0)\)
2. \(\mathbf{2}\) \(1/4,1/4,z\)
3. \(\mathbf{2}'\) \(1/4,1/4,0\)
4. \(\mathbf{2}'\) \(x,1/4,0\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>8 j 2'</td>
<td>x,1/4,1/4 [0,v,w]</td>
<td>x,3/4,1/4 [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 i 2'</td>
<td>1/4,y,1/4 [u,0,w]</td>
<td>3/4 y,1/4 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 h .2</td>
<td>1/4,1/4,z [0,0,w]</td>
<td>3/4,1/4, z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 g .2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0, z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 f 2'</td>
<td>0,y,0 [u,0,w]</td>
<td>0, y,0 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 e 2'</td>
<td>x,0,0 [0,v,w]</td>
<td>x,0,0 [0,v,w]</td>
<td></td>
</tr>
</tbody>
</table>
Asymmetric unit \[0 < x < 1/4; \quad 0 < y < 1/4; \quad 0 < z < 1\]

Symmetry Operations

For \((0,0,0)\) + set

1. \((1) 1 \quad (1,0,0,0)\)
2. \((2) 2 \quad 0,0,z \quad (2,0,0,0)\)
3. \((3) 2’ \quad 0,y,0 \quad (2’,0,0,0)\)
4. \((4) 2’ \quad x,0,0 \quad (2’,0,0,0)\)

For \((0,1/2,1/2)’\) + set

1. \((1) t’ \quad (0,1/2,1/2) \quad (1,0,1/2,1/2)’\)
2. \((2) 2’ (0,0,1/2) 0,1/4,z \quad (2,0,1/2,1/2)’\)
3. \((3) 2’ (0,1/2,0) 0,y,1/4 \quad (2’,0,1/2,1/2)’\)
4. \((4) 2’ (1/4,1/4) \quad x,0,1/4 \quad (2’,0,1/2,1/2)’\)

For \((1/2,0,1/2)’\) + set

1. \((1) t’ (1/2,0,1/2) \quad (1,1/2,0,1/2)’\)
2. \((2) 2’ (0,0,1/2) 1/4,0,z \quad (2,1/2,0,1/2)’\)
3. \((3) 2’ (0,1/2,0) 1/4,y,0 \quad (2’,1/2,0,1/2)’\)
4. \((4) 2’ (1/2,0,0) x,0,1/4 \quad (2’,1/2,0,1/2)’\)

For \((1/2,1/2,0)\) + set

1. \((1) t (1/2,1/2,0) \quad (1,1/2,1/2,0)\)
2. \((2) 2’ 1/4,1/4,z \quad (2,1/2,1/2,0)\)
3. \((3) 2 (0,1/2,0) 1/4,y,0 \quad (2,1/2,1/2,0)\)
4. \((4) 2 (1/2,0,0) x,1/4,0 \quad (2,1/2,1/2,0)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k</td>
<td>(0,0,0) + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 j</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 i</td>
<td>1/4,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>8 e</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>1/4,1/4,3/4 [0,0,w]</td>
</tr>
<tr>
<td>4 c</td>
<td>1/4,1/4,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p 2mm  Along [1,0,0]  p 2mm  Along [0,1,0]  p 2mm
a* = a/2  b* = b/2  a* = c/2  b* = a/2  a* = c/2  b* = a/2
Origin at 1/4,1/4,z  Origin at x,0,0  Origin at 0,y,0
Origin at 22'2'

Asymmetric unit $0 \leq x \leq 1/4$; $0 \leq y \leq 1/4$; $0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) + \text{set}$

1. $1$
2. $2' \ 0,0,z$
3. $2' \ 0,y,0$
4. $2 \ x,0,0$

For $(0,1/2,1/2)' + \text{set}$

1. $1' \ (0,1/2,1/2)$
2. $2 \ (0,0,1/2) \ 0,1/4,z$
3. $2 \ (0,1/2,0) \ 0,y,1/4$
4. $2' \ x,1/4,1/4$

For $(1/2,0,1/2)' + \text{set}$

1. $1' \ (1/2,0,1/2)$
2. $2 \ (0,0,1/2) \ 1/4,0,z$
3. $2 \ 1/4,y,1/4$
4. $2' \ (1/2,0,0) \ x,0,1/4$

For $(1/2,1/2,0)' + \text{set}$

1. $1' \ (1/2,1/2,0)$
2. $2' \ 1/4,1/4,z$
3. $2' \ (0,1/2,0) \ 1/4,y,0$
4. $2 \ (1/2,0,0) \ x,1/4,0$
Continued 22.5.144  

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2)’ +</td>
</tr>
<tr>
<td>16k1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8j2’..</td>
<td>x,1/4,1/4 [0,v,w]</td>
</tr>
<tr>
<td>8i.2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8h.2’</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>8g.2’</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>8f.2’</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>8e2’..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>4d2’2’’</td>
<td>1/4,1/4,3/4 [0,v,0]</td>
</tr>
<tr>
<td>4c2’2’’</td>
<td>1/4,1/4,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4b2’’2’’</td>
<td>0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4a2’’2’’</td>
<td>0,0,0 [u,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p, 2mm</th>
<th>Along [1,0,0]</th>
<th>p₁₂₂, 2mm</th>
<th>Along [0,1,0]</th>
<th>p₁₂₂, 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a/2</td>
<td>b* = b/2</td>
<td>a* = a/2</td>
<td>b* = b/2</td>
<td>a* = a/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,1/4,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,1/4</td>
<td></td>
</tr>
</tbody>
</table>
Orthorhombic
I222 23.1.145

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)
(2) 2  0,0,z
(2_z | 0,0,0)
(3) 2  0,y,0
(2_y | 0,0,0)
(4) 2  x,0,0
(2_x | 0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)
(2) 2  (0,0,1/2)  1/4,1/4,z
(2_z | 1/2,1/2,1/2)
(3) 2  (0,1/2,0)  1/4,y,1/4
(2_y | 1/2,1/2,1/2)
(4) 2  (1/2,0,0)  x,1/4,1/4
(2_x | 1/2,1/2,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 j .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 i .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 h .2</td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 g .2</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 f 2..</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 e 2..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2 d 222</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 c 222</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 222</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 222</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b b* = c</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>c2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c b* = a</td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,0,0

Origin at 0,y,0
I2221' 2221' Orthorhombic
23.2.146

Origin at 2221'

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) $1$ (1 0,0,0)
(2) $2$ 0,0,z (2z 0,0,0)
(3) $2'$ 0,y,0 ($2z'$ 0,0,0)
(4) $2'$ x,0,0 ($2z'$ 0,0,0)

For (1/2,1/2,1/2) + set

(1) $t$ (1/2,1/2,1/2)
(2) $2$ (0,0,1/2) 1/4,1/4,z (2z 1/2,1/2,1/2)
(3) $2$ (0,1/2,0) 1/4,y,1/4 ($2z$ 1/2,1/2,1/2)
(4) $2$ (1/2,0,0) x,1/4,1/4 ($2z$ 1/2,1/2,1/2)

For (0,0,0)'+ set

(1) $t'$ (0,0,0)'
(2) $2'$ 0,0,z ($2z'$ 0,0,0)'
(3) $2'$ 0,y,0 ($2z'$ 0,0,0)'
(4) $2'$ x,0,0 ($2z'$ 0,0,0)'

For (1/2,1/2,1/2)'+ set

(1) $t$ (1/2,1/2,1/2)'
(2) $2'$ (0,0,1/2) 1/4,1/4,z ($2z'$ 1/2,1/2,1/2)'
(3) $2'$ (0,1/2,0) 1/4,y,1/4 ($2z'$ 1/2,1/2,1/2)'
(4) $2'$ (1/2,0,0) x,1/4,1/4 ($2z'$ 1/2,1/2,1/2)'

23.2.146 - 1 - 268
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td></td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
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</table>

8 k 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]
4 j .21' 0,1/2,z [0,0,0] 0,1/2,z [0,0,0]
4 i .21' 0,0,z [0,0,0] 0,0,z [0,0,0]
4 h .21' 1/2,y,0 [0,0,0] 1/2,y,0 [0,0,0]
4 g .21' 0,y,0 [0,0,0] 0,y,0 [0,0,0]
4 f .21' x,0,1/2 [0,0,0] x,0,1/2 [0,0,0]
4 e .21' x,0,0 [0,0,0] x,0,0 [0,0,0]
2 d 2221' 0,1/2,0 [0,0,0]
2 c 2221' 0,0,1/2 [0,0,0]
2 b 2221' 1/2,0,0 [0,0,0]
2 a 2221' 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,0,0] c2mm1' Along [0,1,0] c2mm1'  
\(a^* = a\) \(b^* = b\) \(a^* = b\) \(b^* = c\) \(a^* = c\) \(b^* = a\)
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
I2'2'2 23.3.147

Asymmetric unit
0 < x < 1/2; 0 < y < 1/2; 0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 0,0,0
(2) 2 0,0,z
(3) 2' 0,y,0
(4) 2' x,0,0

(1*) 0,0,0
(2*) 0,0,0
(2*') 0,0,0'
(2*') x,0,0'

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) 1/4,1/4,z
(2) 2 (0,0,1/2) 1/4,1/4,1/4
(3) 2' (0,1/2,0) 1/4,1/4,1/4
(4) 2' (1/2,0,0) x,1/4,1/4

(1*) (1/2,1/2,1/2) 1/2,1/2,1/2
(2*) (0,0,1/2) 1/2,1/2,1/2
(3*) (0,1/2,0) 1/2,1/2,1/2
(4*) (1/2,0,0) 1/2,1/2,1/2
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

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<tr>
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<th>Coordinates</th>
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<tbody>
<tr>
<td>8 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 j .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 i .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 h .2'</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 g .2'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 f 2'..</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 e 2'..</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>2 d 2'2'</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 c 2'2'</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 2'2'</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2 a 2'2'</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm  
Along [1,0,0] c2'mm'  
Along [0,1,0] c2'mm'

a* = a  b* = b
Origin at 0,0,z

a* = -c  b* = b
Origin at x,0,0

a* = c  b* = a
Origin at 0,y,0
Origin at 222

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

For \((0,0,0) + \) set

1. \((1) \begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix}\)
2. \((2) \begin{pmatrix} 0,0,z \\ 0,0,0 \end{pmatrix}\)
3. \((3) \begin{pmatrix} 0,y,0 \\ 0,0,0 \end{pmatrix}\)
4. \((4) \begin{pmatrix} x,0,0 \\ 0,0,0 \end{pmatrix}\)

For \((1/2,1/2,1/2)' + \) set

1. \((1) \begin{pmatrix} 1/2,1/2,1/2 \\ 1/2,1/2,1/2 \end{pmatrix}\)
2. \((2') \begin{pmatrix} 0,0,1/2 \\ 1/4,1/4,z \end{pmatrix}\)
3. \((3) \begin{pmatrix} 0,1/2,0 \\ 1/4,y,1/4 \end{pmatrix}\)
4. \((4) \begin{pmatrix} 1/2,0,0 \\ x,1/4,1/4 \end{pmatrix}\)
Generators selected  
(1); t(1,0,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>k 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>j .2 0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>i .2 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>h .2 1/2,y,0 [0,v,0]</td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>g .2 0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>f 2.. 0,1/2 [u,0,0]</td>
<td>0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>e 2.. 0,0 [u,0,0]</td>
<td>0,0 [u,0,0]</td>
</tr>
<tr>
<td>d 222 0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>c 222 0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>b 222 1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>a 222 0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] cₚ₂m'm'
- Along [1,0,0] cₚ₂m'm'
- Along [0,1,0] cₚ₂m'm'

a* = a  b* = b
Origin at 0,0,z

a* = b  b* = c
Origin at x,0,0

a* = c  b* = a
Origin at 0,y,0
Orthorhombic

Asymmetric unit: $0 \leq x < 1/2; \ 0 \leq y < 1/2; \ 0 \leq z < 1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
2. $2, 0,0,z$
3. $2^\prime, 0,y,0$
4. $2^\prime, x,0,0$

For $(1/2,1/2,1/2)' +$ set

1. $t'(1/2,1/2,1/2)$
2. $2'(0,0,1/2), 1/4,1/4,z$
3. $2(0,1/2,0), 1/4,y,1/4$
4. $2'(1/2,0,0), x,1/4,1/4$
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
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</table>

<table>
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<tr>
<td>8 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 j .2</td>
<td>0,1/2,z [0,0,w] 0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 i .2</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 h .2'</td>
<td>1/2,y,0 [u,0,w] 1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 g .2'</td>
<td>0,y,0 [u,0,w] 0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 f .2'..</td>
<td>x,0,1/2 [0,v,w] x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 e .2'..</td>
<td>x,0,0 [0,v,w] x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>2 d 2'2'</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 c 2'2'</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 2'2'</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2 a 2'2'</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] cₚ 2mm
- Along [1,0,0] cₚ 2'mm
- Along [0,1,0] cₚ 2'mm

**Origin:**
- a* = a  b* = b
- a* = -c  b* = b
- a* = c  b* = a
- Origin at 0,0,z
- Origin at x,0,0
- Origin at 0,y,0
24.1.150

Origin at midpoint of three non-intersecting pairs of parallel 2 axes

Asymmetric unit

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \(1\) \(0,0,0\)
2. \(2\) \((0,0,1/2)\) \(1/4,0,z\)
3. \(2\) \((0,1/2,0)\) \(0,y,1/4\)
4. \(2\) \((1/2,0,0)\) \(x,1/4,0\)

For \((1/2,1/2,1/2) + \text{set}\)

1. \(t\) \((1/2,1/2,1/2)\)
2. \(2\) \((1/2,1/2,1/2)\)
3. \(2\) \((1/2,1/2,1/2)\)
4. \(2\) \((1/2,1/2,1/2)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .2</td>
<td>0,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>4 b .2</td>
<td>1/4,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 a 2..</td>
<td>x,0,1/4 [u,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2m'm'  a* = a  b* = b
Origin at 1/4,0,z

Along [1,0,0]  c2m'm'  a* = b  b* = c
Origin at x,1/4,0

Along [0,1,0]  c2m'm'  a* = c  b* = a
Origin at 0,y,1/4
Origin at midpoint of three non-intersecting pairs of parallel 21' axes

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)  
   \(1 | 0,0,0\)

2. \(2\) \((0,0,1/2)\)  
   \(1/4,0,z\)  
   \((2_z|1/2,0,1/2)\)

3. \(2\) \((0,1/2,0)\)  
   \(0,y,1/4\)  
   \((2_y|0,1/2,1/2)\)

4. \(2\) \((1/2,0,0)\)  
   \(x,1/4,0\)  
   \((2_x|1/2,1/2,0)\)

For \((1/2,1/2,1/2)\) + set

1. \(t\) \((1/2,1/2,1/2)\)  
   \(1/2,1/2,1/2)\)

2. \(2\) \(0,1/4,z\)  
   \((2_z|0,1/2,0)\)

3. \(2\) \(1/4,y,0\)  
   \((2_y|1/2,0,0)\)

4. \(2\) \(x,0,1/4\)  
   \((2_x|0,0,1/2)\)

For \((0,0,0)'\) + set

1. \(1'\)  
   \(1 | 0,0,0)'\)

2. \(2'\) \((0,0,1/2)\)  
   \(1/4,0,z\)  
   \((2_z|1/2,0,1/2)'\)

3. \(2'\) \((0,1/2,0)\)  
   \(0,y,1/4\)  
   \((2_y|0,1/2,1/2)'\)

4. \(2'\) \((1/2,0,0)\)  
   \(x,1/4,0\)  
   \((2_x|1/2,1/2,0)'\)

For \((1/2,1/2,1/2)'\) + set

1. \(t'\) \((1/2,1/2,1/2)'\)  
   \(1/2,1/2,1/2)'\)

2. \(2'\) \(0,1/4,z\)  
   \((2_z|0,1/2,0)'\)

3. \(2'\) \(1/4,y,0\)  
   \((2_y|1/2,0,0)'\)

4. \(2'\) \(x,0,1/4\)  
   \((2_x|0,0,1/2)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

Positions

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<tbody>
<tr>
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<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
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<tr>
<td></td>
<td>(0,0,0)' +</td>
<td>(1/2,1/2,1/2)' +</td>
</tr>
</tbody>
</table>

8  d  11' (1) x,y,z [0,0,0] (2) x+1/2,y+1/2,z+1/2 [0,0,0] (3) x,y+1/2,z+1/2 [0,0,0] (4) x+1/2,y+1/2,z+1/2 [0,0,0]
4  c  .21' 0,1/4,z [0,0,0] 0,3/4,z+1/2 [0,0,0]
4  b  2..1' 1/4,y,0 [0,0,0] 1/4,y,1/2 [0,0,0]
4  a  2..1' x,0,1/4 [0,0,0] x+1/2,0,3/4 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c2mm1'</th>
<th>Along [1,0,0] c2mm1'</th>
<th>Along [0,1,0] c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = c b* = a</td>
</tr>
<tr>
<td>Origin at 1/4,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,1/4</td>
</tr>
</tbody>
</table>
Orthorhombic

24.3.152

I2₁'2₁'2₁

Origin at midpoint of three non-intersecting pairs of parallel 2 and 2’ axes

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 (2) 2 (0,0,1/2) 1/4,0,z (3) 2’ (0,1/2,0) 0,y,1/4 (4) 2’ (1/2,0,0) x,1/4,0

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (2) 2 0,1/4,z (3) 2’ 1/4,y,0 (4) 2’ x,0,1/4

(1) 1 (0,0,0) (2) 1/2,0,1/2 (2) 0,1/2,0 (2) 0,1/2,0 (2) 0,1/2,0

24.3.152 - 1 - 280
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .2</td>
<td>0,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>1/4,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 a 2'</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2mm
  - $a^* = a$, $b^* = b$
- Along [1,0,0] c2'mm'
  - $a^* = -c$, $b^* = b$
- Along [0,1,0] c2'mm'
  - $a^* = c$, $b^* = a$

Origin at 1/4,0,z
Origin at x,1/4,0
Origin at 0,y,1/4
Origin at midpoint of three non-intersecting pairs of parallel 2' axes

Asymmetric unit

\(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0) + \) set

1. \((1) 1\)
2. \((2) 2 (0,0,1/2) \quad 1/4,0,z\)
3. \((3) 2 (0,1/2,0) \quad 0,y,1/4\)
4. \((4) 2 (1/2,0,0) \quad x,1/4,0\)

For \((1/2,1/2,1/2)' + \) set

1. \((1) t' (1/2,1/2,1/2)\)
2. \((2) 2' 0,1/4,z\)
3. \((3) 2' 1/4,y,0\)
4. \((4) 2' x,0,1/4\)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)^*; (2); (3).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
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<tr>
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<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>0,1/4,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,3/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>1/4,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 a 2'..</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,0,3/4 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c\_p,2mm  
 a* = a  b* = b  
Origin at 1/4,0,z

Along [1,0,0]  c\_p,2mm  
 a* = b  b* = c  
Origin at x,1/4,0

Along [0,1,0]  c\_p,2mm  
 a* = c  b* = a  
Origin at 0,y,1/4
Origin at midpoint of three non-intersecting pairs of parallel 2 and 2' axes

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For \((0,0,0) + \) set

\[(1) \ 1 \quad (1 | 0,0,0) \]
\[(2) \ 2 \ (0,0,1/2) \ 1/4,0,z \quad (2 | 1/2,0,1/2) \]
\[(3) \ 2' \ (0,1/2,0) \ 0,y,1/4 \quad (2,1/2,1/2)' \]
\[(4) \ 2' \ (1/2,0,0) \ x,1/4,0 \quad (2,1/2,1/2)' \]

For \((1/2,1/2,1/2)' + \) set

\[(1) \ t' \ (1/2,1/2,1/2) \]
\[(1 | 1/2,1/2,1/2)' \]
\[(2) \ 2' \ 0,1/4,z \quad (2 | 0,1/2,0)' \]
\[(3) \ 2 \ 1/4,y,0 \quad (2,1/2,0,0) \]
\[(4) \ 2 \ x,0,1/4 \quad (2,0,0,1/2) \]
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>8 d 1 (1) x,y,z [u,v,w]</td>
<td>(2) (x+1/2, y, z+1/2 [u,v,w]) (3) (x, y+1/2, z+1/2 [u,v,w]) (4) (x+1/2, y+1/2, z [u,v,w])</td>
</tr>
<tr>
<td>4 c .2' 0,1/4,z [u,v,0]</td>
<td>0,3/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b .2. 1/4,y,0 [0,v,0]</td>
<td>1/4, y, 1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 a 2.. x,0,1/4 [u,0,0]</td>
<td>(x+1/2,0,3/4 [u,0,0])</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c(_{\text{p}})2mm</th>
<th>Along [1,0,0] c(_{\text{p}})2'mm'</th>
<th>Along [0,1,0] c(_{\text{p}})2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mathbf{a}^* = \mathbf{a}) (\mathbf{b}^* = \mathbf{b})</td>
<td>(\mathbf{b}^* = \mathbf{b}) (\mathbf{b}^* = \mathbf{c})</td>
<td>(\mathbf{a}^* = -\mathbf{a}) (\mathbf{b}^* = \mathbf{c})</td>
</tr>
<tr>
<td>Origin at 1/4,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,1/4</td>
</tr>
</tbody>
</table>
Pmm2  mm2  Orthorhombic
25.1.155  Pmm2

Origin on mm2

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

1. $1$
   (1) $1$
   (1) $0,0,0$

2. $2 \cdot 0,0,z$
   (2) $2 \cdot 0,0,0$

3. $m \cdot x,0,z$
   (3) $m \cdot 0,0,0$

4. $m \cdot 0,y,z$
   (4) $m \cdot 0,0,0$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 h m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>2 g m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>2 f .m.</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>2 e .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>1 d mm2</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>1 c mm2</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>1 b mm2</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>1 a mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2mm</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [0,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>a* = b</td>
<td>a* = -a</td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = c</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
**Origin** on mm21'

**Asymmetric unit**

\[
0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1
\]

**Symmetry Operations**

For 1 + set

1. \( \text{Id}(0,0,0) \)
2. \( 2 \ 0,0,z \)
3. \( m \ x,0,z \)
4. \( m \ 0,y,z \)

For 1' + set

1. \( 1' \ (0,0,0)' \)
2. \( 2' \ 0,0,z \)
3. \( m' \ x,0,z \)
4. \( m' \ 0,y,z \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
<td></td>
</tr>
<tr>
<td>4 i 11' (1) x,y,z [0,0,0]</td>
<td>(2) (\overline{x},y,z) [0,0,0]</td>
</tr>
<tr>
<td>2 h m..1' 1/2,y,z [0,0,0]</td>
<td>1/2,(y,z) [0,0,0]</td>
</tr>
<tr>
<td>2 g m..1' 0,y,z [0,0,0]</td>
<td>0,(y,z) [0,0,0]</td>
</tr>
<tr>
<td>2 f .m.1' x,1/2,z [0,0,0]</td>
<td>(x,1/2,z) [0,0,0]</td>
</tr>
<tr>
<td>2 e .m.1' x,0,z [0,0,0]</td>
<td>(x,0,z) [0,0,0]</td>
</tr>
<tr>
<td>1 d mm21' 1/2,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 c mm21' 1/2,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 b mm21' 0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a mm21' 0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2mm1'</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = b)</td>
<td>(b^* = c)</td>
<td>(a^* = -a)</td>
<td>(b^* = c)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Pm'2'm  
m'2'm  
Orthorhombic  

25.3.157  
Pm'2'm  

Asymmetric unit  
0 < x < 1/2;  0 < y < 1/2;  0 < z < 1  

Symmetry Operations  

(1) 1  
(2) 2' 0,0,z  
(3) m x,0,z  
(4) m' 0,y,z  

(1|0,0,0)  
(2|0,0,0)'  
(m|0,0,0)  
(m'|0,0,0)'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>2 h m'..</td>
<td>1/2, y, z [0, v, w]</td>
</tr>
<tr>
<td>2 g m'..</td>
<td>0, y, z [0, v, w]</td>
</tr>
<tr>
<td>2 f .m.</td>
<td>x, 1/2, z [0, v, 0]</td>
</tr>
<tr>
<td>2 e .m.</td>
<td>x, 0, z [0, v, 0]</td>
</tr>
<tr>
<td>1 d m'm2'</td>
<td>1/2, 1/2, z [0, v, 0]</td>
</tr>
<tr>
<td>1 c m'm2'</td>
<td>1/2, 0, z [0, v, 0]</td>
</tr>
<tr>
<td>1 b m'm2'</td>
<td>0, 1/2, z [0, v, 0]</td>
</tr>
<tr>
<td>1 a m'm2'</td>
<td>0, 0, z [0, v, 0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Orthorhombic

25.4.158

Pm'm'2

25.4.158 Pm'm'2

Origin

on m'm'2

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(1 0,0,0)

(2) 2 0,0,z
(2z 0,0,0)

(3) m' x,0,z
(m,0,0,0)

(4) m' 0,y,z
(m,0,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 h m'..</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>2 g m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>2 f .m'</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>2 e .m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>1 d m'm'2</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>1 c m'm'2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>1 b m'm'2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>1 a m'm'2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
P₂c mm² 

25.5.159 

mm²₁’

Orthorhombic

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2|0,0,0)

(3) m x,0,z  
(m|0,0,0)

(4) m 0,y,z  
(m₂|0,0,0)

For (0,0,1)’ + set

(1) t’ (0,0,1)  
(1|0,0,1)’

(2) 2’ (0,0,1) 0,0,z  
(2|0,0,1)’

(3) c’ (0,0,1) x,0,z  
(m₂|0,0,1)’

(4) c’ (0,0,1) 0,y,z  
(m₂|0,0,1)’
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +  (0,0,1)' +</td>
<td></td>
</tr>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 g m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 f .m.</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>4 e .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 d mm2</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 c mm2</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 b mm2</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 a mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p2mm1'  
  \( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)  
  Origin at 0,0,z

- Along [1,0,0] p1m11'  
  \( \mathbf{a}^* = \mathbf{b} \)  \( \mathbf{b}^* = \mathbf{c} \)  
  Origin at x,0,0

- Along [0,1,0] p1m11'  
  \( \mathbf{a}^* = -\mathbf{a} \)  \( \mathbf{b}^* = \mathbf{c} \)  
  Origin at 0,y,0
Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
2. $2 \quad 0,0,z$
3. $m \quad x,0,z$
4. $m \quad 0,y,z$

For $(1,0,0)' + set$

1. $t' (1,0,0)$
2. $2' \quad 1/2,0,z$
3. $a' (1,0,0) \quad x,0,z$
4. $m' \quad 1/2,y,z$

Origin on mm2
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity,</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>Wyckoff letter,</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>(0,0,0) + (1,0,0)'</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 i 1 (1) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h  m'.. 1/2,y,z [0,v,w]</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 g  m.. 0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 f  m.  x,1/2,z [0,v,0]</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>4 e  m.  x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 d  m'm2' 1/2,1/2,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 c  m'm2' 1/2,0,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 b  mm2 0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a  mm2 0,0,z [0,0,0]</td>
<td></td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2a 2mm</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [0,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) ( b^* = b )</td>
<td>( a^* = b ) ( b^* = c )</td>
<td>( a^* = -a ) ( b^* = c )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Asymmetric unit  \(0 \leq x \leq \frac{1}{2};\)  \(0 \leq y \leq \frac{1}{2};\)  \(0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \text{ set}\)

1. \((1) 1(1,0,0)\)
2. \((2) 2(0,0,z)(2z,0,0)\)
3. \((3) m x,0,z(m,0,0)\)
4. \((4) m 0,y,z(m,0,0)\)

For \((1,0,0)' + \text{ set}\)

1. \((1) t' (1,0,0)(1,0,0)'\)
2. \((2) 2' 1/2,0,z(2z,1,0,0)'\)
3. \((3) a'(1,0,0) x,0,z(m,1,0,0)'\)
4. \((4) m' 1/2,y,z(m,1,0,0)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1,0,0) +</td>
</tr>
<tr>
<td>8</td>
<td>i</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
</tr>
<tr>
<td>4</td>
<td>f</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_c 2mm</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Asymmetric unit: $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set:

1. $1$
2. $2', \ 0,0,z$
3. $m, x,0,z$
4. $m', \ 0,y,z$

For $(0,1,0)' +$ set:

1. $t', (0,1,0)$
2. $2', \ 1/2,1/2,z$
3. $m', x,1/2,z$
4. $b'(0,1,0), \ 0,y,z$

Origin is on mm2.
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 g m..</td>
<td>0,y,z [0,u,0]</td>
</tr>
<tr>
<td>4 f .m'.</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4 e .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 d mm2'</td>
<td>1/2,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>2 c mm2</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 b mm2'</td>
<td>0,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>2 a mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p2mm1'</td>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -a</td>
</tr>
<tr>
<td>p1m11'</td>
<td>a* = b</td>
<td>b* = c</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on mm2

**Asymmetric unit** $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

**Symmetry Operations**

For $(0,0,0)$ + set

(1) $t$ $(0,0,0)$
(2) $2 \ 0,0,z$
(3) $m \ x,0,z$
(4) $m \ 0,y,z$

For $(1,0,0)'$ + set

(1) $t' (1,0,0)$
(2) $2' \ 1/2,0,z$
(3) $a' (1,0,0) \ x,0,z$
(4) $m' \ 1/2,y,z$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>8  i  1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4  h  m'..</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>4  g  m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4  f  .m'</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4  e  .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2  d  m'm'2</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2  c  m'm2'</td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>2  b  mm'2'</td>
<td>0,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>2  a  mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2mm1'</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on mm'2'

Asymmetric unit: $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set:

1. $1$
2. $2' \ 0,0,z$
3. $m' \ x,0,z$
4. $m \ 0,y,z$

For $(0,0,1)'$ + set:

1. $t' \ (0,0,1)$
2. $2 \ (0,0,1) \ 0,0,z$
3. $c \ (0,0,1) \ x,0,z$
4. $c' \ (0,0,1) \ 0,y,z$

Orthorhombic
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,0)' +</td>
</tr>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 g m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 f .m'</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4 e .m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>2 d mm'2'</td>
<td>1/2,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>2 c mm'2'</td>
<td>1/2,0,z [u,0,0]</td>
</tr>
<tr>
<td>2 b mm'2'</td>
<td>0,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>2 a mm'2'</td>
<td>0,0,z [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2mm1'</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [0,1,0]</th>
<th>p2v.1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
P2c m'm'2

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1 (2) 2 0,0,z (3) m’ x,0,z (4) m’ 0,y,z
(1|0,0,0) (2z|0,0,0) (m|0,0,0)’ (m|0,0,0)’

For (0,0,1)’ + set

(1) t’ (0,0,1) (2) 2’ (0,0,1) 0,0,z (3) c (0,0,1) x,0,z (4) c (0,0,1) 0,y,z
(1|0,0,1)’ (2z|0,0,1)’ (m|0,0,1) (mz|0,0,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,1)’ +</td>
</tr>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h m’</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 g m’</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 f m’ 3/4</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4 e m’ 3/4</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>2 d m’2</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 c m’2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 b m’2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a m’2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1’  
\( \mathbf{a}^* = \mathbf{a} \)   \( \mathbf{b}^* = \mathbf{b} \)   
Origin at 0,0,z

Along [1,0,0] p211m1’  
\( \mathbf{a}^* = \mathbf{b} \)   \( \mathbf{b}^* = \mathbf{c} \)   
Origin at x,0,0

Along [0,1,0] p211m1’  
\( \mathbf{a}^* = -\mathbf{a} \)   \( \mathbf{b}^* = \mathbf{c} \)   
Origin at 0,y,0
Origin on m'm'2

Asymmetric unit \(0 \leq x \leq 1/2;\) \(0 \leq y \leq 1/2;\) \(0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
   - \((1|0,0,0)\)

2. \(2\)
   - \((0,0,z)\)
   - \((2_z|0,0,0)\)

3. \(m'\)
   - \((x,0,z)\)
   - \((m_y|0,0,0)'\)

4. \(m'\)
   - \((0,y,z)\)
   - \((m_x|0,0,0)'\)

For \((1,0,0)'\) + set

1. \(t'\)
   - \((1,0,0)\)
   - \((1|1,0,0)\)

2. \(2'\)
   - \((1/2,0,z)\)
   - \((2_z|1,0,0)'\)

3. \(a\)
   - \((1,0,0)\)
   - \((x,0,z)\)
   - \((m_y|1,0,0)\)

4. \(m\)
   - \((1/2,y,z)\)
   - \((m_x|1,0,0)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1 (1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1,0,0)' +</td>
</tr>
<tr>
<td>4 h m.. 1/2,y,z [u,0,0]</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 g m'.. 0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 f .m'. x,1/2,z [u,0,w]</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4 e .m'. x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>2 d mm'2' 1/2,1/2,z [u,o,0]</td>
<td></td>
</tr>
<tr>
<td>2 c mm'2' 1/2,0,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b m'm'2 0,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 a m'm'2 0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_{2a}.2m'm'  
\(a^* = a\) \(b^* = b\)  
Origin at 0,0,z

Along [1,0,0]  p_{1m11}  
\(a^* = b\) \(b^* = c\)  
Origin at x,0,0

Along [0,1,0]  p_{2a}.1m1  
\(a^* = -a\) \(b^* = c\)  
Origin at 1/2,y,0
Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \(1\)
   
   \(a\) \((0,0,0)\)

2. \((2)\)
   
   \(b\) \((0,0,0),z\)

3. \((3)\)
   
   \(c\) \((x,0,z)\)

4. \((4)\)
   
   \(d\) \((0,y,z)\)

For \((0,1,0)′ + \text{set}\)

1. \((1)\)
   
   \(a′\) \((0,1,0)\)

2. \((2)′\)
   
   \(b′\) \((0,1/2,z)\)

3. \((3)′\)
   
   \(c′\) \((x,1/2,z)\)

4. \((4)′\)
   
   \(d′\) \((0,y,z)\)
Generators selected \( (1); t(1,0,0); t(0,1,0)^*; t(0,0,1)^*; (2); (3) \).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) ( \bar{x}, \bar{y}, z [\bar{u}, \bar{v}, \bar{w}] )</td>
</tr>
<tr>
<td>4 h m'..</td>
<td>1/2,y,z [0,v,w]</td>
<td>(0,0,0) +</td>
<td>(0,1,0)' +</td>
</tr>
<tr>
<td>4 g m'..</td>
<td>0,y,z [0,v,w]</td>
<td>1/2,( \bar{y}, z [0,\bar{v}, \bar{w}] )</td>
<td></td>
</tr>
<tr>
<td>4 f .m.</td>
<td>x,1/2,z [0,v,0]</td>
<td>( x, \bar{1/2}, z [0,v,0] )</td>
<td></td>
</tr>
<tr>
<td>4 e .m'</td>
<td>x,0,z [u,0,w]</td>
<td>( x, 0, z [u,0,w] )</td>
<td></td>
</tr>
<tr>
<td>2 d m'm2'</td>
<td>1/2,1/2,z [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c m'm2'</td>
<td>1/2,0,z [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b m'm2'</td>
<td>0,1/2,z [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a m'm2'</td>
<td>0,0,z [0,0,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \( p2mm1' \) \( a^* = a \) \( b^* = b \) \( a^* = b \) \( b^* = c \) \( a^* = -a \) \( b^* = c \)
- Origin at \( 0,0,z \) \( Origin \) at \( x,1/2,0 \) \( Origin \) at \( 0,y,0 \)
Origin: on mc2₁

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations:

1. 1
   (0,0,0)

2. 2 (0,0,1/2) 0,0,z
   (0,0,1/2)

3. c (0,0,1/2) x,0,z
   (0,0,1/2)

4. m 0,y,z
   (0,0,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 b m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,z+1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 a m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,z+1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mm  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0]  p1g11'  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [0,1,0]  p_{2v}.1m1  
\( \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at 0,y,0
Origin on mc2,1'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

(1) $1$
   (1) $0,0,0$

(2) $2$ (0,0,1/2) 0,0,z
   (2) $0,0,1/2$

(3) $c$ (0,0,1/2) x,0,z
   (m) $0,0,1/2$

(4) $m$ 0,y,z
   (m) $0,0,0$

For 1' + set

(1) $1'$
   (1) $0,0,0'$

(2) $2'$ (0,0,1/2) 0,0,z
   (2) $0,0,1/2'$

(3) $c'$ (0,0,1/2) x,0,z
   (m') $0,0,1/2'$

(4) $m'$ 0,y,z
   (m') $0,0,0'$
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>1 +</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z+1/2 [0,0,0]</td>
<td>(3) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b m..1'</td>
<td>1/2,y,z [0,0,0]</td>
<td>1/2,y,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a m..1'</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z+1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1'  Along [1,0,0] p1g11'  Along [0,1,0] p1 m11'
\(a^* = a\)  \(b^* = b\)  \(a^* = b\)  \(b^* = c\)  \(a^* = -a\)  \(b^* = c/2\)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on m'c2′

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2′ (0,0,1/2) 0,0,z
(2 | 0,0,1/2)′

(3) c (0,0,1/2) x,0,z
(m | 0,0,1/2)

(4) m′ 0,y,z
(m | 0,0,0)′
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z+1/2 [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 b m'</td>
<td>1/2,y,z [0,v,w] 1/2,y,z+1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 a m'</td>
<td>0,y,z [0,v,w] 0,y,z+1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2’mm’
\[a^* = -b\quad b^* = a\]
Origin at 0,0,z

Along [1,0,0] p1g1
\[a^* = b\quad b^* = c\]
Origin at x,0,0

Along [0,1,0] p2v1m’1
\[a^* = -a\quad b^* = c/2\]
Origin at 0,y,0
Origin on mc'2'_1

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z
(2|0,0,1/2)'

(3) c' (0,0,1/2) x,0,z
(m|0,0,1/2)'

(4) m 0,y,z
(m|0,0,0)
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) ( x,y,z ) ([u,v,w])</td>
<td>( (2) \overline{x},\overline{y},z+1/2 ) ([u,v,w])</td>
<td>( (3) \overline{x},\overline{y},z+1/2 ) ([u,v,w])</td>
</tr>
<tr>
<td>2 b m..</td>
<td>1/2,( y,z ) ([u,0,0])</td>
<td>1/2,( \overline{y},z+1/2 ) ([u,0,0])</td>
<td>( (3) 0,\overline{y},z+1/2 ) ([u,0,0])</td>
</tr>
<tr>
<td>2 a m..</td>
<td>0,( y,z ) ([u,0,0])</td>
<td>0,( \overline{y},z+1/2 ) ([u,0,0])</td>
<td>( (3) 0,\overline{y},z+1/2 ) ([u,0,0])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \( p2'\text{mm}' \) \( a^* = a \quad b^* = b \) \( \text{Origin at } 0,0,z \)  
Along \([1,0,0]\) \( p1\text{g11}' \) \( a^* = b \quad b^* = c \) \( \text{Origin at } x,0,0 \)  
Along \([0,1,0]\) \( p_2\text{v1m1} \) \( a^* = -a \quad b^* = c/2 \) \( \text{Origin at } 0,y,0 \)
Pm'c'2₁  

26.5.172  

m'm'2  

Orthorhombic

Origin on m'c'2₁

Asymmetric unit  
0 < x < 1/2;  0 < y < 1/2;  0 < z < 1

Symmetry Operations

(1) 1  
(1|0,0,0)  

(2) 2  
(2|0,0,1/2)  

(3) c'  
(m,0,0,1/2)  

(4) m'  
(m,0,0,0)  

26.5.172 - 1 - 320
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) \bar{x},\bar{y},z+1/2 [\bar{u},\bar{v},w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,\bar{y},z+1/2 [u,\bar{v},w]</td>
</tr>
<tr>
<td></td>
<td>(4) \bar{x},y,z [\bar{u},v,w]</td>
</tr>
<tr>
<td>2 b m'..</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,\bar{y},z+1/2 [0,v,\bar{w}]</td>
</tr>
<tr>
<td>2 a m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,\bar{y},z+1/2 [0,\bar{v},w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2m'm'
  - Origin at 0,0,z
- Along [1,0,0] p1g'1
  - Origin at \(a^* = a\) \(b^* = b\)
- Along [0,1,0] p2b1m'1
  - Origin at \(x,0,0\)
  - Origin at \(a^* = -a\) \(b^* = c/2\)
Origin on mc₂₁

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0)\) + set

1. \((1)\) 1
   \((1)\) \((0,0,0)\)

2. \((2)\) 2 \((0,0,1/2)\) 0,0,z
   \((2z)\) \((0,0,1/2)\)

3. \((3)\) c \((0,0,1/2)\) \(x,0,z\)
   \((m,y,0,1/2)\)

4. \((4)\) m \(0,y,z\)
   \((m,0,0,0)\)

For \((1,0,0)\)' + set

1. \((1)\) t' \((1,0,0)\)
   \((1)\) \((1,0,0)'\)

2. \((2)\) \(2'\) \((0,0,1/2)\) 1/2,0,z
   \((2z)\) \((1,0,1/2)'\)

3. \((3)\) n' \((1,0,1/2)\) \(x,0,z\)
   \((m,y,1,0,1/2)'\)

4. \((4)\) m' \(1/2,y,z\)
   \((m,1,0,0)'\)
Continued 26.6.173 P₂₃mc2₁

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b m'</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 a m</td>
<td>0,y,z [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>a* = a b* = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>p₂₃.2mm</td>
<td>Origin at 0,0,z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>a* = b b* = c</th>
</tr>
</thead>
<tbody>
<tr>
<td>p₁g11'</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>a* = -a b* = c/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>p₂₃.1m1</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin on mc₂₁

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 (0,0,1/2) \quad 0,0,z \\
(3) & \quad c (0,0,1/2) \quad x,0,z \\
(4) & \quad m \quad 0,y,z \\
\end{align*}
\]

\[
\begin{align*}
(1*) & \quad 0,0,0 \\
(2*) & \quad 0,0,1/2 \\
(m) & \quad 0,0,1/2 \\
(m) & \quad 0,0,0 \\
\end{align*}
\]

For \((0,1,0)\)' + set

\[
\begin{align*}
(1) & \quad t' (0,1,0) \\
(1) & \quad (0,1,0)' \\
(2) & \quad 2' (0,0,1/2) \quad 0,1/2,z \\
(3) & \quad c' (0,0,1/2) \quad x,1/2,z \\
(4) & \quad b' (0,1,0) \quad 0,y,z \\
\end{align*}
\]

\[
\begin{align*}
(1) & \quad (0,0,0)' \\
(2) & \quad (0,0,1/2)' \\
(m) & \quad (0,0,1/2)' \\
(m) & \quad (0,0,0)' \\
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>c</td>
<td>1</td>
</tr>
<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
<td>(2) x̅,y̅,z+1/2 [u̅,v̅,w]</td>
</tr>
<tr>
<td>(2) x̅,y̅,z+1/2 [u̅,v̅,w]</td>
<td>(3) x̅,y̅,z+1/2 [u̅,v̅,w]</td>
<td></td>
</tr>
<tr>
<td>(4) x̅,y̅,z+1/2 [u̅,v̅,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 a m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2₁.2mm  Along [1,0,0]  p1g11'  Along [0,1,0]  p1m11' 
\( \mathbf{a}^* = -\mathbf{b} \)  \( \mathbf{b}^* = \mathbf{a} \)  \( \mathbf{a}^* = \mathbf{b} \)  \( \mathbf{b}^* = \mathbf{c} \)  \( \mathbf{a}^* = -\mathbf{a} \)  \( \mathbf{b}^* = \mathbf{c}/2 \) 
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on \(mc_2\)

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \[1\]
2. \[2\] \((0,0,1/2)\) \(0,0,z\)
3. \[c\] \((0,0,1/2)\) \(x,0,z\)
4. \[m\] \((0,0,1/2)\) \(0,y,z\)

For \((1,0,0)\)' + set

1. \[t'\] \((1,0,0)\)
2. \[2'\] \((0,0,1/2)\) \(1/2,0,z\)
3. \[n'\] \((1,0,1/2)\) \(x,0,z\)
4. \[m'\] \((1,0,0)\) \(1/2,y,z\)

\[26.8.175\]
Generators selected \( (1); t(1,0,0)^{'}; t(0,1,0)^{'}; t(0,0,1); (2); (3). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 ( c ) 1</td>
<td>( (0,0,0) + (1,0,0)^{'} + ) ( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>4 ( b ) ( m^{..} )</td>
<td>( 1/2,y,z [0,v,w] )</td>
</tr>
<tr>
<td>4 ( a ) ( m^{..} )</td>
<td>( 0,y,z [u,0,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \( p_{c2mm} \)
  \( a^* = a \quad b^* = b \)
  Origin at \(0,0,z\)
- Along \([1,0,0]\) \( p_{1g11^{'}*} \)
  \( a^* = b \quad b^* = c \)
  Origin at \(x,0,0\)
- Along \([0,1,0]\) \( p_{1m11^{'}*} \)
  \( a^* = -a \quad b^* = c/2 \)
  Origin at \(0,y,0\)
Origin on mc'2₁⁻¹

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

1. (1 | 0,0,0)
2. (2 | 0,0,1/2) 0,0,z (2' 0,0,1/2) 0,0,z
3. (3 | 0,0,1/2) x,0,z (c' 0,0,1/2) x,0,z
4. (4 | 0,0,0) m 0,y,z (m 0,0,0)

For (1,0,0)' + set

1. (1 | 1,0,0)
2. (2 | 0,0,1/2) 1/2,0,z (2' 0,0,1/2) 1/2,0,z
3. (3 | 1,0,1/2) x,0,z (n 1,0,1/2) x,0,z
4. (4 | 1,0,0)' m' 1/2,y,z (m' 1/2,0,0)

P₂aec'2₁⁻¹  mm21⁻¹  Orthorhombic
Generators selected  \( (1); t(1,0,0)'; t(0,1,0); t(0,0,1); (2); (3). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 8 )</td>
<td>((0,0,0) + (1,0,0)' + )</td>
</tr>
<tr>
<td>( c )</td>
<td>((1) x,y,z [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>((2) x,y,z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>((3) x,y,z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>((4) x,y,z [u,v,w] )</td>
</tr>
</tbody>
</table>

\[ a^* = a \quad b^* = b \]
Origin at \( 1/2,0,z \)
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Projector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along ([0,0,1])</td>
<td>( p_{2a}2m'm' )</td>
</tr>
<tr>
<td>Along ([1,0,0])</td>
<td>( p_{1g}11' )</td>
</tr>
<tr>
<td>Along ([0,1,0])</td>
<td>( p_{2b}.1m1 )</td>
</tr>
</tbody>
</table>

\[ a^* = b \quad b^* = c \]
Origin at \( x,0,0 \)

\[ a^* = c/2 \quad b^* = a \]
Origin at \( 0,y,0 \)
Orthorhombic

**P2₁m'c'2₁**

**mm2₁'**

**Asymmetric unit**

\[ 0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1 \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1\)
2. \(2 (0,0,1/2), 0,0,z\)
3. \(c' (0,0,1/2), x,0,z\)
4. \(m' 0,y,z\)

For \((0,0,0)'\) + set

1. \(t' (0,1,0), 0,0,0\)
2. \(2' (0,0,1/2), 0,1/2,z\)
3. \(c (0,0,1/2), x,1/2,z\)
4. \(b (0,1,0), 0,y,z\)

For \((0,1,0)'\) + set

1. \(t' (0,1,0), 0,0,0\)
2. \(2' (0,1,1/2), 0,1/2,z\)
3. \(c (0,1,1/2), x,1/2,z\)
4. \(b (0,1,0), 0,y,z\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

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<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 b m'</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,z+1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 a m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z+1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_{2a}.2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p_{2a}.1g1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,1/2,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -a</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on cc2

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 $0,0,z$
(2z | 0,0,0)

(3) $c (0,0,1/2) \ x,0,z$
(m, | 0,0,1/2)

(4) $c (0,0,1/2) \ 0,y,z$
(m_\| | 0,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 d .2</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 c .2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 b .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mm  
Along [1,0,0]  p21b1m'1  
Along [0,1,0]  p21b1m'1  

\[ a^* = a \quad b^* = b \]  
Origin at 0,0,0  
\[ a^* = a \quad b^* = c/2 \]  
Origin at x,0,0  
\[ a^* = -a \quad b^* = c/2 \]  
Origin at 0,y,0
Origin: on cc21’

Asymmetric unit: \(0 < x < 1/2; \ 0 < y < 1/2; \ 0 < z \leq 1\)

Symmetry Operations:

For 1 + set:

1. \((1, 0, 0, 0)\)
2. \((2, 0, 0, z)\)
3. \((c, 0, 0, 1/2)\)
4. \((m, 0, 0, 1/2)\)

For 1’ + set:

1. \((1’, 0, 0, 0)’\)
2. \((2’, 0, 0, z)’\)
3. \((c’, 0, 0, 1/2)’\)
4. \((m’, 0, 0, 1/2)’\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>x,y,z [0,0,0]</td>
</tr>
<tr>
<td>2 d ..21'</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c ..21'</td>
<td>1/2,0,z [0,0,0]</td>
<td>1/2,0,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b ..21'</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a ..21'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1'  Along [1,0,0] p1m11'  Along [0,1,0] p1m11'

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Orthorhombic

27.3.180

Pc'c2'

m'm2'

Origin on c'c2'

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

1
(1 | 0,0,0)

2'
(2_ | 0,0,0)^

2c
(3 | 0,0,1/2) x,0,z
(m | 0,0,1/2)

2c'
(4 | 0,0,1/2) 0,y,z
(m_ | 0,0,1/2)
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>e 1 (1) x,y,z [u,v,w] (2) (\bar{x},\bar{y},z [u,v,w]) (3) (x,\bar{y},z+1/2 [\bar{u},v,w]) (4) (\bar{x},y,z+1/2 [\bar{u},v,w])</td>
</tr>
<tr>
<td>2</td>
<td>d .2' 1/2,1/2,z [u,v,0] 1/2,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>c .2' 1/2,0,z [u,v,0] 1/2,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>b .2' 0,1/2,z [u,v,0] 0,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>a .2' 0,0,z [u,v,0] 0,0,z+1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2' mm'
  - \(a^* = -b \quad b^* = a\)
  - Origin at 0,0,z
- Along [1,0,0] p1m1
  - \(a^* = b \quad b^* = c/2\)
  - Origin at x,0,0
- Along [0,1,0] p\(_{2b}\).1m1
  - \(a^* = -a \quad b^* = c/2\)
  - Origin at 0,y,0
Asymmetric unit

\[0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1\]

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \cdot 0,0,z \\
(3) & \quad c' \cdot (0,0,1/2) \cdot x,0,z \\
(4) & \quad c' \cdot (0,0,1/2) \cdot 0,y,z
\end{align*}

\begin{align*}
(1*) & \quad 0,0,0 \\
(2z) & \quad (0,0,0) \\
(my) & \quad (m, 0, 0, 1/2)' \\
(mx) & \quad (m, 0, 0, 1/2)' \end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

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<tr>
<td>4 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 d ..2</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 c ..2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 b ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'  
\( a^* = a \quad b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p1m'1  
\( a^* = b \quad b^* = c/2 \)  
Origin at x,0,0

Along [0,1,0] p1m'1  
\( a^* = -a \quad b^* = c/2 \)  
Origin at 0,y,0
Origin on cc2

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1
(1) $t$ (1,0,0)

(2) $2 \ 0,0,z$
(2) $2'$ $1/2,0,z$

(3) $c (0,0,1/2) \ x,0,z$
(3) $n' (1,0,1/2) \ x,0,z$

(4) $c (0,0,1/2) \ 0,y,z$
(4) $c' (0,0,1/2) \ 1/2,y,z$

For $(1,0,0)'$ + set

(1) $t'$ (1,0,0)
(1) $t'$ (1,0,0)'

(2) $2' \ 1/2,0,z$
(2) $2' \ 1/2,0,z$

(3) $n' (1,0,1/2) \ x,0,z$
(3) $n' (1,0,1/2) \ x,0,z$

(4) $c' (0,0,1/2) \ 1/2,y,z$
(4) $c' (0,0,1/2) \ 1/2,y,z$
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
<td></td>
</tr>
<tr>
<td>8 e 1</td>
<td>(x,y,z [u,v,w])</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 d ..2'</td>
<td>1/2,1/2,z [u,v,0]</td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 c ..2'</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b ..2</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]** p_{2a}.2mm
  
  \[ \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \]
  
  Origin at 0,0,z

- **Along [1,0,0]** p_{1m11}'
  
  \[ \mathbf{a}^* = \mathbf{b}, \mathbf{b}^* = \mathbf{c}/2, \mathbf{c}^* = \mathbf{a} \]
  
  Origin at x,0,0

- **Along [0,1,0]** p_{2a}.1m1
  
  \[ \mathbf{a}^* = -\mathbf{a}, \mathbf{b}^* = \mathbf{c}/2 \]
  
  Origin at 1/2,y,0
Origin on cc2

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0)\) + set

\begin{align*}
(1) & \quad \text{1} \\
(1|0,0,0) & \\
(2) & \quad 0,0,z \\
(2_x|0,0,0) & \\
(3) & \quad c \ (0,0,1/2) \quad x,0,z \\
(m_y|0,0,1/2) & \\
(4) & \quad c \ (0,0,1/2) \quad 0,y,z \\
(m_z|0,0,1/2) & \\
\end{align*}

For \((1,0,0)\)' + set

\begin{align*}
(1) & \quad t' \ (1,0,0) \\
(1|1,0,0)' & \\
(2) & \quad 2' \\
(2_z|1,0,0)' & \\
(3) & \quad n' \ (1,0,1/2) \quad x,0,z \\
(m_y|1,0,1/2)' & \\
(4) & \quad c' \ (0,0,1/2) \\
(m_z|1,0,1/2)' & \\
\end{align*}
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1 ((1) x,y,z \ [u,v,w]) (2) x,y,z+1/2 \ [u,v,w])</td>
<td>((0,0,0)+) ((1,0,0)'+)</td>
</tr>
<tr>
<td>4 d ..2 (1/2,1/2,z \ [0,0,w])</td>
<td>(1/2,1/2,z+1/2 \ [0,0,w])</td>
</tr>
<tr>
<td>4 c ..2' (1/2,0,z \ [u,v,0])</td>
<td>(1/2,0,z+1/2 \ [u,v,0])</td>
</tr>
<tr>
<td>4 a ..2 (0,0,z \ [0,0,w])</td>
<td>(0,0,z+1/2 \ [0,0,w])</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \(p_c\)2mm \(a^*=a \ b^*=b\) Origin at 0,0,z
- Along \([1,0,0]\) \(p1m1\) \(a^*=b \ b^*=c/2\) Origin at x,0,0
- Along \([0,1,0]\) \(p1m1\) \(a^*=-a \ b^*=c/2\) Origin at 0,y,0
Origin on \(c'c2'\)

Asymmetric unit: \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

**Symmetry Operations**

*For \((0,0,0)\) + set*

1. \(1\)
2. \(2'\): \((0,0,0), (0,0,z)
3. \(c\): \((0,0,1/2), (x,0,z)
4. \(c'\): \((0,0,1/2), (0,y,z)

*For \((0,1,0)'\) + set*

1. \(t'\): \((0,1,0), (0,1/2,z)
2. \(2\): \((0,1,0), (0,1/2,z)
3. \(c'\): \((0,0,1/2), (x,1/2,z)
4. \(n\): \((0,1,1/2), (0,y,z)

\(P2\_c'c2'\) mm21' Orthorhombic
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

| 4 d ..2      | 1/2,1/2,z [0,0,w] |
|              | 1/2,1/2,z+1/2 [0,0,w] |

| 4 c ..2'     | 1/2,0,z [u,v,0] |
|              | 1/2,0,z+1/2 [u,v,0] |

| 4 b ..2      | 0,1/2,z [0,0,w] |
|              | 0,1/2,z+1/2 [0,0,w] |

| 4 a ..2'     | 0,0,z [u,v,0] |
|              | 0,0,z+1/2 [u,v,0] |

Symmetry of Special Projections

Along [0,0,1]  p_{2a}.2'mm'  
\( a^* = -b \quad b^* = a \)
Origin at 0,0,z

Along [1,0,0]  p_{2a}.1m1  
\( a^* = b \quad b^* = c/2 \)
Origin at x,0,0

Along [0,1,0]  p_{1m11}'  
\( a^* = -a \quad b^* = c/2 \)
Origin at 0,y,0
Origin on 1a2

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2z | 0,0,0)

(3) a (1/2,0,0) x,0,z
(m_y | 1/2,0,0)

(4) m 1/4,y,z
(m_x | 1/2,0,0)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicities, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>[u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 c m..</td>
<td>1/4,y,z [u,0,0]</td>
<td>[u,0,0]</td>
<td>3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>2 b ..2</td>
<td>0,1/2,z [0,0,w]</td>
<td>[0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td>[0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg

a* = a  b* = b

Origin at 0,0,z

Along [1,0,0] p1m11'

a* = b  b* = c

Origin at x,0,0

Along [0,1,0] p2e1m1

a* = -a/2  b* = c

Origin at 1/4,y,0
Origin on 1a21'

Asymmetric unit  \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1\)

Symmetry Operations

For 1 + set

1. \((1|0,0,0)\)
2. \((2|0,0,z)\)
3. \((a|1/2,0,0)\) \(x,0,z\)
4. \((m|1/4,y,z)\)

For 1' + set

1. \((1'|0,0,0)\)
2. \((2'|0,0,z)\)
3. \((a'|1/2,0,0)\) \(x,0,z\)
4. \((m'|1/4,y,z)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<tbody>
<tr>
<td>4 d 11'</td>
<td>1/4,y,z</td>
<td>(0,0,0)</td>
<td>(2) x, y, z</td>
</tr>
<tr>
<td>2 c m..1'</td>
<td>1/2,1/2,z</td>
<td>(0,0,0)</td>
<td>(3) x+1/2, y, z</td>
</tr>
<tr>
<td>2 b ..21'</td>
<td>0,1/2,z</td>
<td>(0,0,0)</td>
<td>(4) x+1/2, y, z</td>
</tr>
<tr>
<td>2 a ..21'</td>
<td>1/2,0,z</td>
<td>(0,0,0)</td>
<td>(4) x+1/2, y, z</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg1'

\(a^{*} = a\) \(b^{*} = b\)

Origin at 0,0,z

Along [1,0,0] p1m11'

\(a^{*} = b\) \(b^{*} = c\)

Origin at x,0,0

Along [0,1,0] p1m11'

\(a^{*} = -a/2\) \(b^{*} = c\)

Origin at 0,y,0
**Orthorhombic**

Pm'a2'

m'm2'

28.3.187

Pm'a2'

**Origin**
on 1a2'

**Asymmetric unit**

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1

**Symmetry Operations**

(1) 1

(2) 2' 0,0,z

(3) a (1/2,0,0) x,0,z

(4) m' 1/4,y,z

(1 | 0,0,0)

(2 | 0,0,0)'

(m | 1/2,0,0)'

(1/2,0,0)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 c m'..</td>
<td>1/4,y,z [0,v,w]</td>
<td>3/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>2 b ..2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>2 a ..2'</td>
<td>0,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'm'g     Along [1,0,0] p1m11'     Along [0,1,0] p2e,1m1
a* = a    b* = b    a* = b    b* = c    a* = -a/2  b* = c
Origin at 0,0,z          Origin at x,0,0          Origin at 0,y,0
Origin on 1a'2'

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < 1; \quad 0 < z < 1 \]

Symmetry Operations

1. \( 1 \)
   \( (1,0,0,0) \)

2. \( 2' \) \( 0,0,z \)
   \( (2',0,0,0) \)

3. \( a' \) \( (1/2,0,0) \) \( x,0,z \)
   \( (a',1/2,0,0) \)

4. \( m \) \( 1/4,y,z \)
   \( (m,1/2,0,0) \)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

<table>
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<tr>
<td>4  d 1  (1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2  c m..  1/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>2  b .2'  0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>2  a .2'  0,0,z [u,v,0]</td>
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**Symmetry of Special Projections**

<table>
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<tr>
<th>Along [0,0,1] p2'mg'</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [0,1,0] p1m1</th>
</tr>
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<tbody>
<tr>
<td>( \mathbf{a}^* = \mathbf{a} ) ( \mathbf{b}^* = \mathbf{b} )</td>
<td>( \mathbf{a}^* = \mathbf{b} ) ( \mathbf{b}^* = \mathbf{c} )</td>
<td>( \mathbf{a}^* = -\mathbf{a}/2 ) ( \mathbf{b}^* = \mathbf{c} )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin  on 1a'2

Asymmetric unit  $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

Symmetry Operations

(1)  1
    (1 0,0,0)
(2)  2  0,0,z
    (2z 0,0,0)
(3)  a' (1/2,0,0) x,0,z
    (m_x 1/2,0,0')
(4)  m'  1/4,y,z
    (m_y 1/2,0,0')
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 c m'</td>
<td>1/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>2 b .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2m'g' $a^* = a$ $b^* = b$
- Along [1,0,0] p1m'1 $a^* = b$ $b^* = c$
- Along [0,1,0] p1m'1 $a^* = -a/2$ $b^* = c$

Origin at 0,0,z
Origin at x,0,0
Origin at 0,y,0
Orthorhombic

Asymmetric unit: $0 < x < 1/4; \ 0 < y < 1; \ 0 < z < 1$

Symmetry Operations

For $(0,0,0)$ + set:

1. (1) 1
2. (2) 2 \[0,0,z\] 
3. (3) $a (1/2,0,0) \ x,0,z$ 
4. (4) $m \ 1/4,y,z$ 

For $(0,1,0)' + set$:

1. (1) $t' (0,1,0)$ 
2. (2) $2' \ 0,1/2,z$ 
3. (3) $a' (1/2,0,0) \ x,1/2,z$ 
4. (4) $b' (0,1,0) \ 1/4,y,z$ 

Origin on 1a2
Generators selected \( (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3). \)

### Positions

**Multiplicity, Wyckoff letter, Site Symmetry.**

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>( (0,0,0) + (0,1,0)' + )</td>
</tr>
<tr>
<td>4 c m..</td>
<td>(1/4,y,z [u,0,0] )</td>
</tr>
<tr>
<td>4 b ..2'</td>
<td>(0,1/2,z [u,v,0] )</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>(0,0,z [0,0,w] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along \([0,0,1]\) p_{2b-2mg}**
  - \(a^* = a \)
  - \(b^* = b\)
- **Along \([1,0,0]\) p1m11'**
  - \(a^* = b \)
  - \(b^* = c\)
- **Along \([0,1,0]\) p1m11'**
  - \(a^* = -a/2 \)
  - \(b^* = c\)
Origin on 1a2

Asymmetric unit \( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0)\) + set

1. \(I\)
   
2. \(2\) \(0,0,z\)
   
3. \(a\) \((1/2,0,0)\) \(x,0,z\)
   
4. \(m\) \(1/4,y,z\)

For \((0,0,1)\) + set

1. \(t'\) \(0,0,1\)
   
2. \(2'\) \((0,0,1)\) \(0,0,z\)
   
3. \(n'\) \((1/2,0,1)\) \(x,0,z\)
   
4. \(c'\) \((0,0,1)\) \(1/4,y,z\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
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<th>Multiplicity</th>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,1)' +</td>
</tr>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c m..</td>
<td>1/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 b ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mg1'  Along [1,0,0]  p1m11'  Along [0,1,0]  p_c1m1
a* = a  b* = b  a* = b  b* = c  a* = -a/2  b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on 1a2

Asymmetric unit \( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \)  
   \((1 | 0,0,0)\)

2. \((2) \) 0,0,z  
   \((2_z | 0,0,0)\)

3. \((3) a (1/2,0,0) \) x,0,z  
   \((m_y | 1/2,0,0)\)

4. \((4) m \) 1/4,y,z  
   \((m_x | 1/2,0,0)\)

For \((0,1,0)’ + \) set

1. \((1) t’ (0,1,0) \)  
   \((1 | 0,1,0)’\)

2. \((2) \) 0,1/2,z  
   \((2_z | 0,1,0)’\)

3. \((3) a’ (1/2,0,0) \) x,1/2,z  
   \((m_y | 1/2,1,0)’\)

4. \((4) b’ (0,1,0) \) 1/4,y,z  
   \((m_x | 1/2,1,0)’\)
Generators selected  
(1); t(1,0,0); t(0,1,0)'; t(0,0,1)'; (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1,0)' + (1) x,y,z [u,v,w]</td>
<td>(2) $\bar{x}$,$\bar{y}$,$\bar{z}$ [u,$\bar{v}$,$\bar{w}$]</td>
</tr>
<tr>
<td>8 c m.. 1/4,y,z [u,0,0]</td>
<td>3/4,$\bar{y}$,z [u,0,0]</td>
</tr>
<tr>
<td>4 b ..2' 0,1/2,z [u,v,0]</td>
<td>1/2,1/2,z [u,$\bar{v}$,0]</td>
</tr>
<tr>
<td>4 a ..2 0,0,z [0,0,0]</td>
<td>1/2,0,z [0,0,$\bar{w}$]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p2mg1'</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [0,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbf{a}^* = \mathbf{a}$ $\mathbf{b}^* = \mathbf{b}$</td>
<td>$\mathbf{a}^* = \mathbf{b}$ $\mathbf{b}^* = \mathbf{c}$</td>
<td>$\mathbf{a}^* = -\mathbf{a}/2$ $\mathbf{b}^* = \mathbf{c}$</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
*Orthorhombic*

28.9.193

**Origin** on 1a2'

**Asymmetric unit**

\[ 0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \(1\)
   
   \((1|0,0,0)\)

2. \(2'\)
   
   \((2'z|0,0,0)^{'}\)

3. \(a\)
   
   \((m_y|1/2,0,0)\)

4. \(m'\)
   
   \((m_x|1/2,0,0)^{'}\)

For \((0,1,0)^{'} + \text{set}\)

1. \(t'\)
   
   \((1|0,1,0)^{'}\)

2. \(2\)
   
   \((2z|0,1,0)\)

3. \(a'\)
   
   \((m_y|1/2,1,0)^{'}\)

4. \(b\)
   
   \((m_x|1/2,1,0)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>4</td>
<td>(0,1,0)′ +</td>
</tr>
</tbody>
</table>

Site Symmetry:

- 8 d 1: x,y,z [u,v,w]
- (2) x, y, z [u,v,w]
- (3) x+1/2, y, z [u,v,w]
- (4) x+1/2, y, z [u,v,w]

- 4 c m′: 1/4, y, z [0,v,w]
- 3/4, y, z [0,v,w]

- 4 b .2: 0,1/2, z [0,0,w]
- 1/2, 1/2, z [0,0,w]

- 4 a .2: 0,0, z [u,v,0]
- 1/2, 0, z [u,v,0]

Symmetry of Special Projections

Along [0,0,1]  p_{2b}.2m′g′

- a* = a  b* = b
- Origin at 0,1/2,z

Along [1,0,0]  p_{2a}.1m1

- a* = b  b* = c
- Origin at x,0,0

Along [0,1,0]  p1m11′

- a* = -a/2  b* = c
- Origin at 0,y,0
Orthorhombic

28.10.194

P₂c m'a₂'

mm21'

Origin on 1a₂'

Asymmetric unit  
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2' 0,0,z
(2|0,0,0)'

(3) a (1/2,0,0)  x,0,z
(m_y|1/2,0,0)

(4) m' 1/4,y,z
(m_x|1/2,0,0)'

For (0,0,1)' + set

(1) t' (0,0,1)
(1|0,0,1)'

(2) 2 (0,0,1) 0,0,z
(2|0,0,1)

(3) n' (1/2,0,1)  x,0,z
(m_y|1/2,0,1)'

(4) c (0,0,1)  1/4,y,z
(m_x|1/2,0,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (0,0,1) +</td>
</tr>
<tr>
<td>8 d 1 (1) x,y,z [u,v,w]</td>
<td>(2) ( \bar{x},y,z [u,v,w] ) (3) ( x+1/2,y,z [u,v,w] ) (4) ( x+1/2,y,z [\bar{u},v,w] )</td>
</tr>
<tr>
<td>4 c m' 1/4,y,z [0,v,w]</td>
<td>3/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 b ..2' 0,1/2,z [u,v,0]</td>
<td>1/2,1/2,z [\bar{u},v,0]</td>
</tr>
<tr>
<td>4 a ..2' 0,0,z [u,v,0]</td>
<td>1/2,0,z [\bar{u},v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) p2mg1'  
Along \([1,0,0]\) p2\(\text{b}^*\)1m1  
Along \([0,1,0]\) p\(\text{c}^*\)1m1

\(\mathbf{a}^* = \mathbf{a}\)  \(\mathbf{b}^* = \mathbf{b}\)  
\(\mathbf{a}^* = \mathbf{b}\)  \(\mathbf{b}^* = \mathbf{c}\)  
\(\mathbf{a}^* = -\mathbf{a}/2\)  \(\mathbf{b}^* = \mathbf{c}\)

Origin at \(0,0,z\)  
Origin at \(x,0,0\)  
Origin at \(0,y,0\)
Origin on $1a'2'$

Asymmetric unit $0 \leq x \leq 1/4; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1
(1) 1
(1) 0,0,0)

(2) 2' 0,0,z
(2) $0,0,0'$
(2) 0,0,0)

(3) $a' (1/2,0,0) \ x,0,z$
(3) $a' (1/2,0,0)'$
(3) $a' (1/2,0,0)'$

(4) m 1/4,y,z
(4) m 1/4,y,z
(4) m 1/4,y,z

For $(0,0,1)'$ + set

(1) t' (0,0,1)
(1) t' (0,0,1)'
(1) 0,0,1)

(2) 2 (0,0,1) 0,0,z
(2) $0,0,1$)
(2) $0,0,1$)

(3) n (1/2,0,1) x,0,z
(3) n (1/2,0,1)
(3) n (1/2,0,1)

(4) c' (0,0,1) 1/4,y,z
(4) c' (0,0,1)'
(4) c' (0,0,1)'

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Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>8  d 1 (1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4  c m.. 1/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>4  b ..2' 0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4  a ..2' 0,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg1'  
\( a^* = a \quad b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p1m11'  
\( a^* = b \quad b^* = c \)  
Origin at x,0,0

Along [0,1,0] p2v,1m1  
\( a^* = -a/2 \quad b^* = c \)  
Origin at 0,y,0
Origin on 1a'2

Asymmetric unit \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) +\) set

\[
\begin{align*}
(1) & \quad 1 \\
(1') & \quad (0,0,0) \\
(2) & \quad 0,0,z \\
(2') & \quad (0,0,0)
\end{align*}
\]

\[
\begin{align*}
(3) & \quad a'(1/2,0,0) \quad x,0,z \\
(3') & \quad (1/2,0,0)'
\end{align*}
\]

\[
\begin{align*}
(4) & \quad m' \quad 1/4,y,z \\
(4') & \quad (1/2,0,0)'
\end{align*}
\]

For \((0,0,1) +\) set

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(1') & \quad (0,0,1)'
\end{align*}
\]

\[
\begin{align*}
(2) & \quad 2' \quad (0,0,1) \quad 0,0,z \\
(2') & \quad (0,0,1)'
\end{align*}
\]

\[
\begin{align*}
(3) & \quad n \quad (1/2,0,1) \quad x,0,z \\
(3') & \quad (1/2,0,1)
\end{align*}
\]

\[
\begin{align*}
(4) & \quad c \quad (0,0,1) \quad 1/4,y,z \\
(4') & \quad (1/2,0,1)
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity,  Coordinates
Wyckoff letter,  (0,0,0) + (0,0,1)' +
Site Symmetry.

<table>
<thead>
<tr>
<th>d</th>
<th>(1)</th>
<th>(2)</th>
<th>(3)</th>
<th>(4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>x+1/2,y,z [u,v,w]</td>
<td>x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>1/4,y,z [0,v,w]</td>
<td>3/4,y,z [0,v,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mg1'    Along [1,0,0]  p2v,1m1'     Along [0,1,0]  p2v,1m1
a* = a     b* = b    a* = b     b* = c    a* = -a/2   b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on 1a'2

Asymmetric unit

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

1. \((1, 0, 0, 0)\)
2. \((2, 0, 0, z)\)
3. \(a'(1/2, 0, 0)\) \(x, 0, z\)
4. \(m'1/4, y, z\)

For \((0,1,0)'\) + set

1. \((1', 0, 1, 0)\)
2. \((2', 0, 1/2, z)\)
3. \(a(1/2, 0, 0)\) \(x, 1/2, z\)
4. \(b(0, 1, 0)\) \(1/4, y, z\)
**Generators selected**  
(1); t(1,0,0); t(0,1,0)'; t(0,0,1)'; (2); (3).

**Positions**

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<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c m'..</td>
<td>1/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 b ..2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  p2mg1'  
\[ \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0]  p_{1}^{1}m1  
\[ \mathbf{a}^* = \mathbf{b}, \mathbf{b}^* = \mathbf{c} \]
Origin at x,1/2,0

Along [0,1,0]  p1m11'  
\[ \mathbf{a}^* = -\mathbf{a}/2, \mathbf{b}^* = \mathbf{c} \]
Origin at 0,y,0
Origin on 1a2₁

Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1

Symmetry Operations:

1. 1
   (1 | 0,0,0)
2. x,0,z
   (m | 1/2,0,0)
3. 0,0,z
   (0,0,1/2)
4. 1/4,y,z
   (m | 1/2,0,1/2)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>4 a 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2b*-1m1
a* = b  b* = c/2
Origin at x,0,0

Along [0,1,0] p2a*-1g1
a* = -a/2  b* = c
Origin at 1/4,y,0
Origin on 1a₁₂₁'

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

Symmetry Operations

For 1 + set

1

(1) 1
(1) 0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2) 0,0,1/2)

(3) a (1/2,0,0) x,0,z
(3) m y,1/2,0,0)

(4) c (0,0,1/2) 1/4,y,z
(4) m z,1/2,0,1/2)

For 1' + set

1'

(1) 1'
(1) 0,0,0)

(2) 2' (0,0,1/2) 0,0,z
(2) 0,0,1/2)

(3) a' (1/2,0,0) x,0,z
(3) m y,1/2,0,0)

(4) c' (0,0,1/2) 1/4,y,z
(4) m z,1/2,0,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a 1'</td>
</tr>
<tr>
<td>1'</td>
<td>(1) x, y, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2, y, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2, y, z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mg1'  
\( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0]  p1m11'  
\( \mathbf{a}^* = \mathbf{b} \)  \( \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at x,0,0

Along [0,1,0]  p1g11'  
\( \mathbf{a}^* = -\mathbf{a}/2 \)  \( \mathbf{b}^* = \mathbf{c} \)  
Origin at 0,y,0
Pc'a2',

29.3.200

m'm2'

Pc'a2',

Orthorhombic

Origin on 1a2',

Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z
(2z|0,0,1/2')

(3) a (1/2,0,0) x,0,z
(m|1/2,0,0)

(4) c' (0,0,1/2) 1/4,y,z
(m|1/2,0,1/2')
Generators selected  \((1)\); \(t(1,0,0); t(0,1,0); t(0,0,1)\); \((2)\); \((3)\).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 a 1</td>
<td>(1) (x,y,z) ([u,v,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) p2m'g'  
\(a^* = a\) \(\quad b^* = b\) 
Origin at 0,0,z

Along \([1,0,0]\) p1m1  
\(a^* = b\) \(\quad b^* = c/2\) 
Origin at x,0,0

Along \([0,1,0]\) p2a*1g1  
\(a^* = -a/2\) \(\quad b^* = c\) 
Origin at 0,y,0
Origin on 1a'2,'

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1  
   (1 0,0,0)  
   (1 |0,0,0)

(2) 2' (0,0,1/2) 0,0,z  
   (2 0,0,1/2')

(3) a' (1/2,0,0) x,0,z  
   (m 1/2,0,0')

(4) c (0,0,1/2) 1/4,y,z  
   (m 1/2,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 a 1 (1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x̄,ȳ,z+1/2 [u,v̅,w̅]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y,z [u,v̅,w̅]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z+1/2 [u,v̅,w̅]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mg'  
\( a^* = a \)  \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p2b*1m'1  
\( a^* = b \)  \( b^* = c/2 \)  
Origin at x,0,0

Along [0,1,0] p1g'1  
\( a^* = -a/2 \)  \( b^* = c \)  
Origin at 0,y,0
Origin on $1a'2_1$

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) 1  
(1 | 0,0,0)  

(2) 2 (0,0,1/2) 0,0,z  
(2z | 0,0,1/2)  

(3) $a'$ (1/2,0,0) x,0,z  
(m_y | 1/2,0,0)'  

(4) $c'$ (0,0,1/2) 1/4,y,z  
(m_x | 1/2,0,1/2)'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

4 a 1

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(3) x+1/2,y,z [u,v,w]</td>
<td>(4) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'g'
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p1m'1
\( a^* = b \quad b^* = c/2 \)
Origin at x,0,0

Along [0,1,0] p1g'1
\( a^* = -a/2 \quad b^* = c \)
Origin at 0,y,0
Origin on 1a2₁

Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z
    (2|0,0,1/2)

(3) a (1/2,0,0) x,0,z
    (mₚ|1/2,0,0)

(4) c (0,0,1/2) 1/4,y,z
    (mₚ|1/2,0,1/2)

For (0,1,0)’ + set

(1) t’ (0,1,0)
   (1|0,1,0)’

(2) 2’ (0,0,1/2) 0,1/2,z
    (2|₀,0,1/2)’

(3) a’ (1/2,0,0) x,1/2,z
    (mₚ|1/2,1,0)’

(4) n’ (0,1,1/2) 1/4,y,z
    (mₚ|1/2,1,1/2)’
Generators selected  (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
(0,0,0) &+ (0,1,0)'+ \quad (0,0,0) &+ (0,1,0)' + \\
8 \quad a \quad 1 &\quad (1) x,y,z [u,v,w] &\quad (2) \bar{x},\bar{y},z+1/2 [\bar{u},\bar{v},w] &\quad (3) x+1/2,y,z [u,v,\bar{w}] &\quad (4) \bar{x}+1/2,y,z+1/2 [u,\bar{v},\bar{w}]
\end{align*}
\]

Symmetry of Special Projections

Along [0,0,1]  p2₁ca₂₁  Along [1,0,0]  p₁c₁m₁  Along [0,1,0]  p₁g₁₁'

\[
\begin{align*}
a^* &= a & b^* &= b & a^* &= a/2 & b^* &= c & a^* &= -a/2 & b^* &= c
\end{align*}
\]

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on 1a’2₁

Asymmetric unit \( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0) + \text{ set}\)

1. \((1)\) 1
2. \((2)\) \(2 (0,0,1/2) \quad 0,0,z \quad (2_1) (0,0,1/2)
3. \((3)\) a’ \((1/2,0,0) \quad 1/2,x,z \quad (m_y | 1/2,0,0)’
4. \((4)\) c’ \((0,0,1/2) \quad 1/4,y,z \quad (m_z | 1/2,0,1/2)’

For \((0,1,0)^+ \text{ set}\)

1. \((1)\) t’ \((0,1,0) \quad (1) | 0,1,0)’
2. \((2)\) \(2’ (0,0,1/2) \quad 0,1/2,z \quad (2_1) (0,1,1/2)’
3. \((3)\) a \((1/2,0,0) \quad 1/2,x,z \quad (m_y | 1/2,1,0)
4. \((4)\) n \((0,1,1/2) \quad 1/4,y,z \quad (m_z | 1/2,1,1/2)’

\(P_{2b} c'a'2_1\) mm21' Orthorhombic

29.7.204

\(P_{2b} c'a'2_1\)
Generators selected: (1); t(1,0,0); t(0,1,0)'; t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[(0,0,0) + (0,1,0)' + \]

| 8 | a | 1 | \( (1) x, y, z \) \([u,v,w]\) | \( (2) x, y, z+1/2 \) \([u,v,w]\) | \( (3) x+1/2, y, z \) \([u,v,w]\) | \( (4) x+1/2, y+1/2, z \) \([u,v,w]\) |

Symmetry of Special Projections

Along \([0,0,1]\) \( p_{2b}-2m'g' \)  
\( a^* = a \) \( b^* = b \)  
Origin at 0,0,z

Along \([1,0,0]\) \( p_{2a}.1m1 \)  
\( a^* = b \) \( b^* = c/2 \)  
Origin at x,1/2,0

Along \([0,1,0]\) \( p1g11' \)  
\( a^* = -a/2 \) \( b^* = c \)  
Origin at 0,y,0
Origin on n12

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1 
   (1 | 0,0,0)
(2) 2 0,0,z 
   (2z | 0,0,0)
(3) c (0,0,1/2) x,1/4,z 
   (m,0,1/2,1/2)
(4) n (0,1/2,1/2) 0,y,z 
   (m,0,1/2,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 b .2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 a .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg

Origin at 0,0,z

a* = -b  b* = a
Origin on n121'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set

1. $1$  
2. $2 \quad 0,0,z$  
3. $c \quad (0,0,1/2) \quad x,1/4,z$  
4. $n \quad (0,1/2,1/2) \quad 0,y,z$

For 1' + set

1'. $1'$  
2'. $2' \quad 0,0,z$  
3'. $c' \quad (0,0,1/2) \quad x,1/4,z$  
4'. $n' \quad (0,1/2,1/2) \quad 0,y,z$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 +</td>
<td>1' +</td>
</tr>
<tr>
<td>4 c 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) (\bar{x},\bar{y},z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) (x,\bar{y}+1/2,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) (\bar{x},y+1/2,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td>2 b .21'</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a .21'</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2mg1'</th>
<th>Along [1,0,0]</th>
<th>c1m11'</th>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = -b)</td>
<td>(b^* = a)</td>
<td>(a^* = b)</td>
<td>(b^* = c)</td>
<td>(a^* = -a)</td>
<td>(b^* = c/2)</td>
</tr>
</tbody>
</table>
Origin on n'12'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $1$
   \[ (1) (0,0,0) \]
2. $2'$
   \[ (2) 0,0,z \quad (2_z) 0,0,0' \]
3. $c$
   \[ (3) (0,0,1/2) \quad x,1/4,z \quad (m_y) 0,1/2,1/2 \]
4. $n'$
   \[ (4) (n') (0,1/2,1/2) \quad 0,y,z \quad (m_x) 0,1/2,1/2' \]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>c 1</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 2'</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 2'</td>
</tr>
<tr>
<td></td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2'mg'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p_{2v,1m1}</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -a</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on n12'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1
(2) 2' 0,0,z
(3) c' (0,0,1/2) x,1/4,z
(4) n (0,1/2,1/2) 0,y,z

(1*) 0,0,0
(2*) 0,0,0)
(3*) (0,0,1/2)*
(4*) (0,1/2,1/2)*
Generators selected: \( t(1,0,0); t(0,1,0); t(0,0,1); (2); (3) \).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) ( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>2 b ..2'</td>
<td>1/2,0,( z [u,v,0] )</td>
</tr>
<tr>
<td>2 a ..2'</td>
<td>0,0,( z [u,v,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2'm'g</th>
<th>Along [1,0,0]</th>
<th>c(_p),1m1</th>
<th>Along [0,1,0]</th>
<th>p1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{a} = -\mathbf{b} \quad \mathbf{b} = \mathbf{a} )</td>
<td>( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} )</td>
<td>( \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,( z )</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on n’12

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

\[
\begin{align*}
(1) & \quad \begin{cases} 1 \quad (1,0,0) \\ z \quad (0,0,0) \end{cases} \\
(2) & \quad 0,0,z \\
(3) & \quad c’ (0,0,1/2) \\
(4) & \quad n’ (0,1/2,1/2) \\
\end{align*}
\]
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<th>Multiplicity</th>
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<tr>
<td>4 c 1</td>
<td>(1) ( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(2) ( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(3) ( x,y+1/2,z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(4) ( x,y+1/2,z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td>2 b ..2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2m'g'
  - \( a^* = -b \quad b^* = a \)
  - Origin at 0,0,z

- Along [1,0,0] c1m'1
  - \( a^* = b \quad b^* = c \)
  - Origin at x,0,0

- Along [0,1,0] p1m1
  - \( a^* = -a \quad b^* = c/2 \)
  - Origin at 0,y,0
Orthorhombic

Asymmetric unit

\[0 < x < 1/2; \quad 0 < y < 1; \quad 0 < z < 1/2\]

Symmetry Operations

For \((0,0,0) + \) set

(1) \(1\) \hspace{1cm} (2) \(2\) \hspace{1cm} (3) \(c\) \hspace{1cm} (4) \(n\)

\[
\begin{align*}
(1) & \ (0,0,0) \\
(2) & \ (0,0,z) \\
(3) & \ (0,0,1/2) \\
(4) & \ (0,1/2,1/2)
\end{align*}
\]

(1*) \(0,0,0\) \hspace{1cm} (2*) \(0,0,0\) \hspace{1cm} (m*) \(0,1/2,1/2\) \hspace{1cm} (m*) \(0,1/2,1/2\)

For \((1,0,0) + \) set

(1) \(t'\) \hspace{1cm} (2) \(2'\) \hspace{1cm} (3) \(n'\) \hspace{1cm} (4) \(n'\)

\[
\begin{align*}
(1) & \ (1,0,0) \\
(2) & \ (1/2,0,z) \\
(3) & \ (1,0,1/2) \\
(4) & \ (0,1/2,1/2)
\end{align*}
\]

(1*) \(1,0,0\) \hspace{1cm} (2*) \(1,0,0\) \hspace{1cm} (m*) \(1,1/2,1/2\) \hspace{1cm} (m*) \(1,1/2,1/2\)

For \((1,0,0)' + \) set

(1) \(t'\) \hspace{1cm} (2) \(2'\) \hspace{1cm} (3) \(n'\) \hspace{1cm} (4) \(n'\)

\[
\begin{align*}
(1) & \ (1,0,0)' \\
(2) & \ (1/2,0,z) \\
(3) & \ (1,0,1/2) \\
(4) & \ (0,1/2,1/2)
\end{align*}
\]

(1*) \(1,0,0\)' \hspace{1cm} (2*) \(1,0,0\)' \hspace{1cm} (m*) \(1,1/2,1/2\) \hspace{1cm} (m*) \(1,1/2,1/2\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p21-2mg
a* = -b  b* = a
Origin at 0,0,z

Along [1,0,0] c1m11'
a* = b  b* = c
Origin at x,0,0

Along [0,1,0] p_c1m1
a* = -a  b* = c/2
Origin at 1/2,y,0
**Origin**  
on n12'

**Asymmetric unit**  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

1. (1) 1  
   (1 0,0,0)

2. (2') 0,0,z  
   (2'z 0,0,0)'

3. (3) c' (0,0,1/2)  
   x,1/4,z  
   (m_y 0,1/2,1/2)'

4. (4) n (0,1/2,1/2)  
   y,z  
   (m_x 0,1/2,1/2)

For (1,0,0)' + set

1. (1) t' (1,0,0)  
   (1 1,0,0)'

2. (2) 1/2,0,z  
   (2z 1,0,0)

3. (3) n (1,0,1/2)  
   x,1/4,z  
   (m_y 1,1/2,1/2)'

4. (4) n' (0,1/2,1/2)  
   1/2,y,z  
   (m_x 1,1/2,1/2)'
Generators selected  
\[(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).\]

Positions  

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) ( \bar{x}, \bar{y}, z [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(3) ( x, y+1/2, z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(4) ( \bar{x}, y+1/2, z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td>4 b ..2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections  

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>( p_{2a}.2m'g' )</th>
<th>Along [1,0,0]</th>
<th>( c1m11' )</th>
<th>Along [0,1,0]</th>
<th>( p_{2a}.1m1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = -b )</td>
<td>( b^* = a )</td>
<td>( a^* = b )</td>
<td>( b^* = c )</td>
<td>( a^* = -a )</td>
<td>( b^* = c/2 )</td>
</tr>
<tr>
<td>Origin at 1/2,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Pmn$_2_1$

31.1.212

mm2

Pmn$_2_1$

Orthorhombic

Origin on mn1

Asymmetric unit

$0 \leq x \leq 1/2;$  $0 \leq y \leq 1/2;$  $0 \leq z \leq 1$

Symmetry Operations

(1) $1$

(1 | 0,0,0)

(2) $2$ (0,0,1/2)  1/4,0,z

(2z | 1/2,0,1/2)

(3) $n$ (1/2,0,1/2)  x,0,z

(m | 1/2,0,1/2)

(4) $m$  0,y,z

(m,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

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<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>4 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 a m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2, y,z+1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2mg</th>
<th>Along [1,0,0]</th>
<th>p1g11'</th>
<th>Along [0,1,0]</th>
<th>c_{p1}1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a) (b^* = b)</td>
<td>(a^* = b) (b^* = c)</td>
<td>(a^* = -a) (b^* = c)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 1/4,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on mn11'

Asymmetric unit 0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1

Symmetry Operations

For 1 + set

\begin{align*}
(1) & \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\
(2) & \begin{pmatrix} 2 \end{pmatrix} (0,0,1/2) 1/4,0,z \\
& \text{(2) } (2z | 1/2,0,1/2) \\
\end{align*}

\begin{align*}
(3) & \begin{pmatrix} n \end{pmatrix} (1/2,0,1/2) x,0,z \\
& \text{(3) } (m_{y} | 1/2,0,1/2) \\
\end{align*}

\begin{align*}
(4) & \begin{pmatrix} m \end{pmatrix} 0,y,z \\
& \text{(4) } (m_{x} | 0,0,0) \\
\end{align*}

For 1’ + set

\begin{align*}
(1) & \begin{pmatrix} 1 \end{pmatrix} \\
(1) & \begin{pmatrix} 1' \end{pmatrix} \\
\end{align*}

\begin{align*}
\begin{pmatrix} 2' \end{pmatrix} (0,0,1/2) 1/4,0,z \\
& \text{(2) } (2z | 1/2,0,1/2) \\
\end{align*}

\begin{align*}
\begin{pmatrix} n' \end{pmatrix} (1/2,0,1/2) x,0,z \\
& \text{(3) } (m_{y} | 1/2,0,1/2) \\
\end{align*}

\begin{align*}
\begin{pmatrix} m' \end{pmatrix} 0,y,z \\
& \text{(4) } (m_{x} | 0,0,0) \\
\end{align*}
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'. \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1 + 1' + )</td>
<td></td>
</tr>
<tr>
<td>( 4 \quad b \quad 11' )</td>
<td>( (1) \ x,y,z \ [0,0,0] )</td>
</tr>
<tr>
<td></td>
<td>( (2) \ x+1/2, y,z+1/2 \ [0,0,0] )</td>
</tr>
<tr>
<td></td>
<td>( (3) x+1/2, y,z+1/2 \ [0,0,0] )</td>
</tr>
<tr>
<td></td>
<td>( (4) x,y,z \ [0,0,0] )</td>
</tr>
<tr>
<td>( 2 \quad a \quad m..1' )</td>
<td>( 0,y,z \ [0,0,0] )</td>
</tr>
<tr>
<td></td>
<td>( 1/2, y,z+1/2 \ [0,0,0] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along \([0,0,1]\)  \( \text{p2mg}1' \)  
  \( \mathbf{a}^* = a \quad \mathbf{b}^* = b \)  
- Along \([1,0,0]\)  \( \text{p1g}11' \)  
  \( \mathbf{a}^* = b \quad \mathbf{b}^* = c \)  
- Along \([0,1,0]\)  \( \text{c1m}11' \)  
  \( \mathbf{a}^* = -a \quad \mathbf{b}^* = c \)
Origin on \( m'n1 \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

\( Pm'n2_1' \)

\( m'm2' \)

Orthorhombic

\[ 31.3.214 \]

\[ Pm'n2_1' \]

\[ 31.3.214 \]

\[ Pm'n2_1' \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

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<tr>
<td>4 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2, y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 a m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2, y,z+1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mg'       Along [1,0,0] p1g1   Along [0,1,0] c_p-1m`1
a* = a   b* = b       a* = b   b* = c   a* = -a   b* = c
Origin at 1/4,0,z          Origin at x,0,0    Origin at 0,y,0
Pmn'2_1'  

mm'2'  

Orthorhombic  

31.4.215  
Pmn'2_1'  

Origin on mn'1  

Asymmetric unit  

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1  

Symmetry Operations  

(1) 1  
(1 | 0,0,0)  

(2) 2' (0,0,1/2) 1/4,0,z  
(2_z | 1/2,0,1/2)  

(3) n' (1/2,0,1/2) x,0,z  
(m_y | 1/2,0,1/2)  

(4) m 0,y,z  
(m_x | 0,0,0)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2, y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 a m..</td>
<td>0,y,z [u,0,0]</td>
<td>1/2, y,z+1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mg'  Along [1,0,0] p1g11'  Along [0,1,0] c1m1

\( a^* = a \quad b^* = b \)

Origin at 1/4,0,z

\( a^* = b \quad b^* = c \)

Origin at x,0,0

\( a^* = -a \quad b^* = c \)

Origin at 0,y,0
Origin on m'\n'1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) 1

(2) $2 (0,0,1/2) \quad 1/4,0,z$

(3) $n' (1/2,0,1/2) \quad x,0,z$

(4) $m' \quad 0,y,z$

$\left(m,1/2,0,1/2\right)'$

$\left(m,0,0,0\right)'$
Continued

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, 
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 a m'3</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,z+1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'g'  
Along [1,0,0] p1g'1  
Along [0,1,0] c1m1

<table>
<thead>
<tr>
<th>a' = a</th>
<th>b' = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = b</td>
<td>b' = c</td>
</tr>
<tr>
<td>a' = -a</td>
<td>b' = c</td>
</tr>
</tbody>
</table>

Origin at 1/4,0,z  
Origin at x,0,0  
Origin at 0,y,0
Orthorhombic

31.6.217

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 1
(1) t'
(1) t'

(2) 2 (0,0,1/2) 1/4,0,z
(2') (0,0,1/2) 1/4,1/2,z
(2) 2' (0,0,1/2) 1/4,1/2,z
(2' (0,0,1/2) 1/2,1/2,z

(3) n (1/2,0,1/2) x,0,z
(3) n' (1/2,0,1/2) x,1/2,z
(3) n' (1/2,0,1/2) x,1/2,z
(3) n' (1/2,0,1/2) x,1/2,z

(4) m 0,y,z
(4) m 0,y,z
(4) m 0,y,z
(4) m 0,y,z

For (0,1,0)' + set

(1) 0,1,0)
(1) 0,1,0)
(1) 0,1,0)
(1) 0,1,0)

(2) 2 (0,0,1/2) 1/4,0,z
(2') (0,0,1/2) 1/4,1/2,z
(2) 2' (0,0,1/2) 1/4,1/2,z
(2' (0,0,1/2) 1/2,1/2,z

(3) n (1/2,0,1/2) x,0,z
(3) n' (1/2,0,1/2) x,1/2,z
(3) n' (1/2,0,1/2) x,1/2,z
(3) n' (1/2,0,1/2) x,1/2,z

(4) m 0,y,z
(4) m 0,y,z
(4) m 0,y,z
(4) m 0,y,z
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

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<tbody>
<tr>
<td>8 b 1</td>
<td>(0,0,0) + (0,1,0) +</td>
</tr>
<tr>
<td>4 a m.. 0,y,z [u,0,0]</td>
<td>1/2, y,z+1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p$_{21}$.mg
- Along [1,0,0] p1g11'
- Along [0,1,0] c1m11'

- a$^*$ = a  b$^*$ = b
- a$^*$ = b  b$^*$ = c
- a$^*$ = -a  b$^*$ = c
Orthorhombic

P₂ｂｍ'n2₁¹

mm2¹

31.7.218

P₂ｂｍ'n2₁¹

Origin on m'n1

Asymmetric unit
0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 0,0,0)

(2) 2' (0,0,1/2) 1/4,0,z
(2_z 1/2,0,1/2)'

(3) n (1/2,0,1/2) x,0,z
(m_y 1/2,0,1/2)

(4) m' 0,y,z
(m_x 0,0,0)'

For (0,1,0)' + set

(1) t' (0,1,0)
(1 0,1,0)'

(2) 2 (0,0,1/2) 1/4,1/2,z
(2_z 1/2,1,1/2)

(3) n' (1/2,0,1/2) x,1/2,z
(m_y 1/2,1,1/2)'

(4) b (0,1,0) 0,y,z
(m_x 0,1,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

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<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 a m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_{2a}.2m'g'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 1/4,1/2,z

Along [1,0,0]  p_{2a}'1g1  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [0,1,0]  c_{1m11}'  
\( \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c} \)  
Origin at 0,y,0
Pba2  mm2  Orthorhombic

32.1.219  Pba2

Origin  on 112

Asymmetric unit  \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1\)

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1 \| 0,0,0) & \\
(2) & \quad 0,0,z \\
(2 \| 0,0,0) & \\
(3) & \quad a (1/2,0,0) \quad x,1/4,z \\
(m \| 1/2,0,0) & \\
(4) & \quad b (0,1/2,0) \quad 1/4,y,z \\
(m \| 1/2,1/2,0) & 
\end{align*}
\]
Generators selected  
(1); \(t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

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<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td>2 b ..2</td>
<td>0,1/2,(z [0,0,w])</td>
</tr>
<tr>
<td>2 a ..2</td>
<td>0,0,(z [0,0,w])</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\)  \(p2gg\)  
  \(a^* = a\)  \(b^* = b\)  
  Origin at 0,0,\(z\)

- Along \([1,0,0]\)  \(p_{2a^*1m1}\)  
  \(a^* = b/2\)  \(b^* = c\)  
  Origin at x,1/4,0

- Along \([0,1,0]\)  \(p_{2a^*1m1}\)  
  \(a^* = c/2\)  \(b^* = c\)  
  Origin at 1/4,y,0
Origin on 1121'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For 1 + set

(1) 1
   (1|0,0,0)

(2) 2 0,0,z
    (2|0,0,0)

(3) a (1/2,0,0) x,1/4,z
    (m|1/2,1/2,0)

(4) b (0,1/2,0) 1/4,y,z
    (m|1/2,1/2,0)

For 1' + set

(1) 1'
   (1|0,0,0)'

(2) 2' 0,0,z
    (2|0,0,0)'

(3) a' (1/2,0,0) x,1/4,z
    (m|1/2,1/2,0)'

(4) b' (0,1/2,0) 1/4,y,z
    (m|1/2,1/2,0)'

Pba21' mm21' Orthorhombic
32.2.220 Pba21'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1'</td>
<td></td>
</tr>
</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>4</th>
<th>1'</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
<td>(3) x+1/2, y+1/2, z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>1/2, 1/2, z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>1/2, 1/2, z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg1' Along [1,0,0] p1m11' Along [0,1,0] p1m11'
\(a^* = a\) \(b^* = b\) \(a^* = b/2\) \(b^* = c\) \(a^* = -a/2\) \(b^* = c\)

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Pb'a2'  m'm2'  Orthorhombic
32.3.221  Pb'a2'

Origin  on 112'

Asymmetric unit  0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
    (1|0,0,0)

(2) 2' 0,0,z
    (2|0,0,0)'

(3) a (1/2,0,0)  x,1/4,z
    (m,|1/2,1/2,0)

(4) b' (0,1/2,0)  1/4,y,z
    (m,|1/2,1/2,0)'

32.3.221 - 1 - 418
**Generators selected**  \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 ( c )</td>
<td>( (1) \ x, y, z \ [u, v, w] )</td>
</tr>
<tr>
<td>2 ( b )</td>
<td>( 0,1/2, z \ [u, v, 0] )</td>
</tr>
<tr>
<td>2 ( a )</td>
<td>( 0,0, z \ [u, v, 0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \( p2'gg' \)
- \( a^* = -b \quad b^* = a \)
- Origin at \(0,0,z\)

- Along \([1,0,0]\) \( p1m1 \)
- \( a^* = b/2 \quad b^* = c \)
- Origin at \(x,0,0\)

- Along \([0,1,0]\) \( p_{2a',1m1} \)
- \( a^* = -a/2 \quad b^* = c \)
- Origin at \(0,y,0\)
Origin on 112

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

(1) 1
(2) 2   0,0,z
(3) a' (1/2,0,0)   x,1/4,z
(4) b' (0,1/2,0)   1/4,y,z

\( (m_y|1/2,1/2,0) \quad (m_x|1/2,1/2,0) \)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2, y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2, y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>2 b ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 a ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2g'g'  
Along [1,0,0] p_{2a'1m1}  
Along [0,1,0] p_{2a'1m1}  

\( a^* = a \quad b^* = b \)  
\( a^* = b/2 \quad b^* = c \)  
\( a^* = -a/2 \quad b^* = c \)  

Origin at 0,0,z  
Origin at x,0,0  
Origin at 1/4,y,0
Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
   $(1|0,0,0)$

2. $2$ $0,0,z$
   $(2|0,0,0)$

3. $a$ $(1/2,0,0)$ $x,1/4,z$
   $(m_y|1/2,1/2,0)$

4. $b$ $(0,1/2,0)$ $1/4,y,z$
   $(m_x|1/2,1/2,0)$

For $(0,0,1)' +$ set

1. $t'$ $(0,0,1)$
   $(1|0,0,1)'$

2. $2'$ $(0,0,1)$ $0,0,z$
   $(2|0,0,1)'$

3. $n'$ $(1/2,0,1)$ $x,1/4,z$
   $(m_y|1/2,1/2,1)'$

4. $n'$ $(0,1/2,1)$ $1/4,y,z$
   $(m_x|1/2,1/2,1)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{array}{cccccc}
\text{Multiplicity} & \text{Wyckoff letter} & \text{Site Symmetry} \\
8 & c & 1 & (1) x, y, z [u, v, w] & (2) \bar{x}, y, z [\bar{u}, v, w] & (3) x+1/2, y+1/2, z [u, v, w] & (4) \bar{x}+1/2, \bar{y}+1/2, z [u, v, w] \\
4 & b & .2 & 0, 1/2, z [0, 0, w] & 1/2, z [0, 0, w] \\
4 & a & .2 & 0, 0, z [0, 0, w] & 1/2, 1/2, z [0, 0, w] \\
\end{array}
\]

Symmetry of Special Projections

Along [0,0,1] \( p2gg' \)  Along [1,0,0] \( p_{c1} \)  Along [0,1,0] \( p_{c1} \)
\( a^* = a \quad b^* = b \)  \( a^* = b/2 \quad b^* = c \)  \( a^* = -a/2 \quad b^* = c \)
Origin at 0,0,z  Origin at x,1/4,0  Origin at 1/4,y,0
P$_{2c}$ b'a2' mm21' Orthorhombic 32.6.224 P$_{2c}$ b'a2'

Origin on 112'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2' 0,0,z
(3) a (1/2,0,0) x,1/4,z
(4) b' (0,1/2,0) 1/4,y,z

For (0,0,1)' + set

(1) t' (0,0,1)
(2) 2 (0,0,1) 0,0,z
(3) n' (1/2,0,1) x,1/4,z
(4) n (0,1/2,1) 1/4,y,z
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x, y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2, y+1/2, z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2, y+1/2, z [u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

| 4 b ..2'     | 0,1/2, z [u,v,0] |
|              | 1/2,0, z [u,v,0] |

| 4 a ..2'     | 0,0, z [u,v,0] |
|              | 1/2,1/2, z [u,v,0] |

Symmetry of Special Projections

Along [0,0,1]  p2gg1'  Along [1,0,0]  pab1m1  Along [0,1,0]  pc1m1

<table>
<thead>
<tr>
<th>a* = a</th>
<th>b* = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>a* = -a/2</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
P_2c b'a'2
32.7.225
Orthorhombic

mm21'
P_2c b'a'2

Origin on 112

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z
(3) a' (1/2,0,0) x,1/4,z
(4) b' (0,1/2,0) 1/4,y,z

For (0,0,1)' + set

(1) t' (0,0,1)
(2) 2' (0,0,1) 0,0,z
(3) n (1/2,0,1) x,1/4,z
(4) n (0,1/2,1) 1/4,y,z

(1') (0,0,0)
(2') (0,0,0)
(3') (1/2,1/2,0)
(4') (1/2,1/2,0)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td></td>
<td>(0,0,1)’ +</td>
<td></td>
</tr>
<tr>
<td>8 c 1</td>
<td>x,y,z [u,v,w]</td>
<td>x+1/2, y+1/2,z [u,v,w]</td>
<td>p2gg1’</td>
</tr>
<tr>
<td>4 b .2</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
<td>p 2b<em>1m</em>1</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>p 2b<em>1m</em>1</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2gg1’</th>
<th>Along [1,0,0]</th>
<th>p 2b<em>1m</em>1</th>
<th>Along [0,1,0]</th>
<th>p 2b<em>1m</em>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = b/2)</td>
<td>(b^* = c)</td>
<td>(a^* = -a/2)</td>
<td>(b^* = c)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>
Origin on 112₁

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 (0,0,1/2) 0,0,z

(2₂ | 0,0,1/2)

(3) a (1/2,0,0) x,1/4,z

(4) n (0,1/2,1/2) 1/4,y,z

(m₁ | 1/2,1/2,1/2)
Continued

Generators selected  (1); \(t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).\)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 a 1</td>
<td>(1) x,y,z [u,v,w]  (2) (\bar{x},\bar{y},z+1/2 [\bar{u},\bar{v},w])  (3) (x+1/2, y+1/2, z [u,v,w])  (4) (\bar{x}+1/2, y+1/2, z+1/2 [u,v,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg  Along [1,0,0] c\(_1\)m1  Along [0,1,0] p\(_2\)g1
\(a^* = a\)  \(b^* = b\)  \(a^* = b\)  \(b^* = c\)  \(a^* = -a/2\)  \(b^* = c\)
Origin at 0,0,z  Origin at x,1/4,0  Origin at 1/4,y,0
Origin on 112,1′

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $1 +$ set

(1) 1
(1′ | 0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2′x | 0,0,1/2)

(3) a (1/2,0,0) x,1/4,z
(my | 1/2,1/2,0)

(4) n (0,1/2,1/2) 1/4,y,z
(mz | 1/2,1/2,1/2)

For $1′ +$ set

(1) 1′
(1′ | 0,0,0)′

(2) 2′ (0,0,1/2) 0,0,z
(2′x | 0,0,1/2)′

(3) a′ (1/2,0,0) x,1/4,z
(my′ | 1/2,1/2,0)′

(4) n′ (0,1/2,1/2) 1/4,y,z
(mz′ | 1/2,1/2,1/2)′

Pna2,1′

33.2.227

mm21′

Pna2,1′

Orthorhombic
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'. \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>1' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4  a  11'</td>
<td>(1) x,y,z [0,0,0] (2) ( \bar{x}, \bar{y}, z+1/2 ) [0,0,0] (3) ( x+1/2, \bar{y}+1/2, z ) [0,0,0] (4) ( \bar{x}+1/2, y+1/2, z+1/2 ) [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) ( b^* = b )</td>
<td>p2gg1'</td>
<td>c1m11'</td>
<td>p1g11'</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 112,$\bar{1}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) $1$

(2') $(0,0,1/2) \quad 0,0,z$

(2) $2' \quad (0,0,1/2)'$

(3) $a \quad (1/2,0,0) \quad x,1/4,z$

(4) $n' \quad (0,1/2,1/2) \quad 1/4,y,z$

(3) $a \quad (1/2,0,0) \quad x,1/4,z$

(4) $m \quad (1/2,1/2,0)$

(4') $m' \quad (1/2,1/2,1/2)'$
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 a 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2'gg'
  - a* = -b
  - b* = a
- Along [1,0,0] c1m1
  - a* = b
  - b* = c
- Along [0,1,0] p2a.1g1
  - a* = -a/2
  - b* = c

Origin at 0,0,z
Origin at x,1/4,0
Origin at 0,y,0
**Origin** on 112₁⁺

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

1. \( 1 \)
   - \((1, 0, 0, 0)\)

2. \( 2' \)
   - \((0, 0, 1/2, 0, 0, z)\)
   - \((0, 0, 1/2, 0, 0, z)\)'

3. \( a' \)
   - \((1/2, 0, 0, x, 1/4, z)\)
   - \((1/2, 0, 0, x, 1/4, z)\)'

4. \( n \)
   - \((0, 1/2, 1/2, 1/4, y, z)\)
   - \((0, 1/2, 1/2, 1/4, y, z)\)'

\[ 33.4.229 \]

Pna'2₁⁺ mm'2⁺ Orthorhombic
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

4  a  1  (1) x,y,z [u,v,w]  (2) x,y,z+1/2 [u,v,w]  (3) x+1/2,y+1/2,z [u,v,w]  (4) x+1/2,y+1/2,z+1/2 [u,v,w]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Special Projection</th>
<th>a*</th>
<th>b*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p2'gg'</td>
<td>a = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>c,1m1</td>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Along [0,1,0]</td>
<td>p1g1</td>
<td>a* = -a/2</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z Origin at x,1/4,0 Origin at 0,y,0
Origin on 112₁

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(2) 2 (0,0,1/2) 0,0,z
(3) a’ (1/2,0,0) x,1/4,z
(4) n’ (0,1/2,1/2) 1/4,y,z

(1₁ 0,0,0)
(2₂ 0,0,1/2)
(mₙ 1/2,1/2,0)'
(mₘ 1/2,1/2,1/2)'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>a 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x, y, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+1/2, y+1/2, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2g'g'  
Along [1,0,0]  c1m'1  
Along [0,1,0]  p1g'1

a* = a  b* = b  
a* = b  b* = c  
a* = -a/2  b* = c  

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at 0,y,0
Origin on 112

Asymmetric unit: $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations:

1. $1$
   - $(1 \ 0,0,0)$
2. $2$
   - $(0,0,z)$
   - $(z,0,0)$
3. $n$
   - $(1/2,0,1/2) x,1/4,z$
   - $(m_y,1/2,1/2,1/2)$
4. $n$
   - $(0,1/2,1/2) 1/4,y,z$
   - $(m_z,1/2,1/2,1/2)$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x+1/2,y+1/2,z+1/2 [u,v,w] (4) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 b ..2</td>
<td>0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a ..2</td>
<td>0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2gg</th>
<th>Along [1,0,0]</th>
<th>c_p1m1</th>
<th>Along [0,1,0]</th>
<th>c_p1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
<td>a^* = b</td>
<td>b^* = c</td>
<td>a^* = -a</td>
<td>b^* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
**Origin** on 1121'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

For \(1\) + set

1. \((1)\) 0,0,0
2. \((2)\) 0,0,z
3. \((3)\) (1/2,0,1/2) x,1/4,z
4. \((4)\) (0,1/2,1/2) 1/4,y,z

For \(1'\) + set

1. \((1')\) 0,0,0
2. \((2')\) 0,0,z
3. \((3')\) (1/2,0,1/2) x,1/4,z
4. \((4')\) (0,1/2,1/2) 1/4,y,z
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>1' +</td>
</tr>
<tr>
<td>4 c 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>2 b .21'</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 a .21'</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2gg1'</th>
<th>Along [1,0,0]</th>
<th>c1m11'</th>
<th>Along [0,1,0]</th>
<th>c1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = -a b* = c</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on 112'

Asymmetric unit $0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1$

Symmetry Operations

(1) 1
(1) 0,0,0

(2) $2'$ 0,0,z
(2) $2'_{x}$ 0,0,0'

(3) $n (1/2,0,1/2)$ $x,1/4,z$
(3) $m_{y} (1/2,1/2,1/2)$

(4) $n' (0,1/2,1/2)$ 1/4,y,z
(4) $m_{x} (1/2,1/2,1/2)'$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>2</td>
<td>0,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2'gg'</th>
<th>Along [1,0,0]</th>
<th>c1m1</th>
<th>Along [0,1,0]</th>
<th>c_p,1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b  b* = a</td>
<td>a* = b  b* = c</td>
<td>a* = -a  b* = c</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0


Origin on 112

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2 | 0,0,0)

(3) \(n'\ (1/2,0,1/2)\) \(x,1/4,z\)
(m_\perp | 1/2,1/2,1/2)'

(4) \(n'\ (0,1/2,1/2)\) \(1/4,y,z\)
(m_\perp | 1/2,1/2,1/2)'
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x+1/2,y+1/2,z+1/2 [u,v,w] (4) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>2 b .2</td>
<td>0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a .2</td>
<td>0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2g'g'  Along [1,0,0]  c,p,1m'1  Along [0,1,0]  c1m'1
a* = a  b* = b  a* = b  b* = c  a* = -a  b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on 112

Asymmetric unit:

- $0 \leq x \leq 1/2$;
- $0 \leq y \leq 1/2$;
- $0 \leq z \leq 1$

Symmetry Operations:

For $(0,0,0)$ + set:

1. $t$ $(0,0,0)$
2. $2^1 (0,0,0)$
3. $d (1/2,0,1/2) x,1/4,z$
4. $d (0,1/2,1/2) 1/4,y,z$

For $(1,0,0)' + set$:

1. $t' (1,0,0)$
2. $2' (1/2,0,1/2) x,1/4,z$
3. $d' (3/2,0,1/2) x,1/4,z$
4. $d' (0,1/2,1/2) 3/4,y,z$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(0,0,0) + (1,0,0) +</td>
</tr>
<tr>
<td>4 b ..2</td>
<td>0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2gg1'  
  \( a^* = a \quad b^* = b \)
- Along [1,0,0] c1m11'  
  \( a^* = b \quad b^* = c \)
- Along [0,1,0] c1m11'  
  \( a^* = -a \quad b^* = c \)
- Origin at 0,0,z  
  Origin at x,0,0  
  Origin at 0,y,0
Asymmetric unit: \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) +\) set

1. \(t\) \((0,0,0)\)
2. \(2 \quad 0,0,z\)
3. \(m \quad x,0,z\)
4. \(m \quad 0,y,z\)

For \((1/2,1/2,0) +\) set

1. \(t\) \((1/2,1/2,0)\)
2. \(2 \quad 1/4,1/4,z\)
3. \(a \quad (1/2,0,0) \quad x,1/4,z\)
4. \(b \quad (0,1/2,0) \quad 1/4,y,z\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>8 f 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m.. 0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 d .m. x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 c ..2 1/4,1/4,z [0,0,w]</td>
<td>1/4,3/4,z [0,0,w]</td>
</tr>
<tr>
<td>2 b mm2 0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a mm2 0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along 0,0,1</th>
<th>c2mm</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = -a/2</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,0,0

Origin at 0,y,0
Asymmetric unit \(0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2_z) & \quad 0,0,0 \\
(3) & \quad m \quad x,0,z \\
(3_m) & \quad (m_y,0,0) \\
(4) & \quad m \quad 0,y,z \\
(4_m) & \quad (m_y,0,0) \\
\end{align*}
\]

For \((1/2,1/2,0)\) + set

\[
\begin{align*}
(1) & \quad t \quad 1/2,1/2,0 \\
(1) & \quad (1/2,1/2,0) \\
(2) & \quad 2 \quad 1/4,1/4,z \\
(2_z) & \quad 1/2,1/2,0 \\
(3) & \quad a \quad (1/2,0,0) \quad x,1/4,z \\
(3_m) & \quad (m_y,1/2,1/2,0) \\
(4) & \quad b \quad (0,1/2,0) \quad 1/4,y,z \\
(4_m) & \quad (m_y,1/2,1/2,0) \\
\end{align*}
\]

For \((0,0,0)\)' + set

\[
\begin{align*}
(1) & \quad 1' \\
(1) & \quad (0,0,0)' \\
(2) & \quad 2' \quad 0,0,z \\
(2_z) & \quad 0,0,0)' \\
(3) & \quad m' \quad x,0,z \\
(3_m) & \quad (m_y,0,0)' \\
(4) & \quad m' \quad 0,y,z \\
(4_m) & \quad (m_y,0,0)' \\
\end{align*}
\]

For \((1/2,1/2,0)\)' + set

\[
\begin{align*}
(1) & \quad t' \quad 1/2,1/2,0 \\
(1) & \quad (1/2,1/2,0)' \\
(2) & \quad 2' \quad 1/4,1/4,z \\
(2_z) & \quad 1/2,1/2,0)' \\
(3) & \quad a' \quad (1/2,0,0) \quad x,1/4,z \\
(3_m) & \quad (m_y,1/2,1/2,0)' \\
(4) & \quad b' \quad (0,1/2,0) \quad 1/4,y,z \\
(4_m) & \quad (m_y,1/2,1/2,0)' \\
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' + (0,0,0)'

8 f 11' (1) x,y,z [0,0,0] (2) x',y,z [0,0,0] (3) x',y,z [0,0,0] (4) x',y,z [0,0,0]

4 e m.,1' 0,y,z [0,0,0] 0,y,z [0,0,0]

4 d m.,1' x,0,z [0,0,0] x,0,z [0,0,0]

4 c ..21' 1/4,1/4,z [0,0,0] 1/4,3/4,z [0,0,0]

2 b mm1' 0,1/2,z [0,0,0] 0,1/2,z [0,0,0]

2 a mm1' 0,0,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,0,0] p1m11' Along [0,1,0] p1m11'

\[ a^* = a \quad b^* = b \] \[ a^* = b/2 \quad b^* = c \] \[ a^* = -a/2 \quad b^* = c \]

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Asymmetric unit  

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0) + \text{set}\):

- (1) 1
- (2) \(2'\) 0,0,z
- (3) \(m\) x,0,z
- (4) \(m'\) 0,y,z

For \((1/2,1/2,0) + \text{set}\):

- (1) \(t\) (1/2,1/2,0)
- (2) \(2'\) 1/4,1/4,z
- (3) \(a\) (1/2,0,0) x,1/4,z
- (4) \(b'\) (0,1/2,0) 1/4,y,z
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions
Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 d .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 c ..2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>2 b m'm2'</td>
<td>0,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>2 a m'm2'</td>
<td>0,0,z [0,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2mm'
  - \(a^* = -b\) \(b^* = a\)
  - Origin at 0,0,z

- Along [1,0,0] p1m1
  - \(a^* = b/2\) \(b^* = c\)
  - Origin at x,0,0

- Along [0,1,0] p1m11'
  - \(a^* = -a/2\) \(b^* = c\)
  - Origin at 0,y,0
Asymmetric unit

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0) + \) set

1. \((1|0,0,0)\)
2. \((2|0,0,z)\)
3. \((m'|x,0,z)\)
4. \((m'|0,y,z)\)

For \((1/2,1/2,0) + \) set

1. \((t|1/2,1/2,0)\)
2. \((2|1/4,1/4,z)\)
3. \((a'|1/2,0,0)\)
4. \((b'|0,1/2,0)\)

\((1|1/2,1/2,0)\)
\((2|1/2,1/2,0)\)
\((m|1/2,1/2,0)'\)
\((m_s|1/2,1/2,0)'\)
Generators selected  \( (1) \ t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3). \)

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

\[
\begin{array}{cccc}
\text{Positions} & \text{Coordinates} & \text{Multiplicity} & \text{Wyckoff letter} \\
& \text{Site Symmetry} & \text{(0,0,0)} & \text{(1/2,1/2,0)} \\
(0,0,0) + (1/2,1/2,0) + & \text{(2)} x,y,z [u,v,w] & 8 & f \\
& \text{(3)} x,y,z [u,v,w] & 4 & e \text{m'} \cdot \\
& \text{(4)} x,y,z [u,v,w] & 4 & d \text{.m'} \\
& \text{(5)} x,y,z [u,v,w] & 4 & c \text{.2} \\
& \text{(6)} x,y,z [u,v,w] & 2 & b \text{m'} m' \cdot \\
& \text{(7)} x,y,z [u,v,w] & 2 & a \text{m'} m' \cdot \\
\end{array}
\]

Symmetry of Special Projections

\[
\begin{array}{ccc}
\text{Along [0,0,1]} & \text{c2m'} & \text{Along [1,0,0]} & \text{p1m'} & \text{Along [0,1,0]} & \text{p1m'} \\
\text{a}^* = a & \text{b}^* = b & \text{a}^* = b/2 & \text{b}^* = c & \text{a}^* = -a/2 & \text{b}^* = c \\
\text{Origin at 0,0,z} & \text{Origin at x,0,0} & \text{Origin at 0,y,0} \\
\end{array}
\]

35.4.239 - 2 - 455
Origin on mm2

Asymmetric unit: $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

(1) $t\quad (0,0,0)$
(2) $2\quad 0,0,z$
(3) $m\quad x,0,z$
(4) $m\quad 0,y,z$

For $(1/2,1/2,0)$ + set

(1) $t\quad (1/2,1/2,0)$
(2) $2\quad 1/4,1/4,z$
(3) $a\quad (1/2,0,0)\quad x,1/4,z$
(4) $b\quad (0,1/2,0)\quad 1/4,y,z$

For $(0,0,1)'$ + set

(1) $t'\quad (0,0,1)'$
(2) $2'\quad (0,0,1)\quad 0,0,z$
(3) $c'\quad (0,0,1)\quad x,0,z$
(4) $c'\quad (0,0,1)'\quad 0,y,z$

For $(1/2,1/2,1)'$ + set

(1) $t'\quad (1/2,1/2,1)'$
(2) $2'\quad (0,0,1)\quad 1/4,1/4,z$
(3) $n'\quad (1/2,0,1)\quad x,1/4,z$
(4) $n'\quad (0,1/2,1)\quad 1/4,y,z$
Generators selected  
(1); t(1,0,0); t(0,0,1); t(0,0,1)'; t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 d .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 c ..2</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>4 b mm2</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 a mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1]  
  c2mm1'  
  \( \mathbf{a}^* = \mathbf{a} \), \( \mathbf{b}^* = \mathbf{b} \)  
  Origin at 0,0,z

- Along [1,0,0]  
  p1m11'  
  \( \mathbf{a}^* = \mathbf{b}/2 \), \( \mathbf{b}^* = \mathbf{c} \)  
  Origin at x,0,0

- Along [0,1,0]  
  p1m11'  
  \( \mathbf{a}^* = -\mathbf{a}/2 \), \( \mathbf{b}^* = \mathbf{c} \)  
  Origin at 0,y,0
Asymmetric unit: $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) + \text{ set}$

1. $1$
   
   $$(1) \begin{cases} 1 & (0,0,0) \\ (1) & (0,0,0) \end{cases}$$

2. $2$
   
   $$(2) \begin{cases} 2 & 0,0,z \\ (2_z) & 0,0,0 \end{cases}$$

3. $m$
   
   $$(3) \begin{cases} m & x,0,z \\ (m_y) & 0,0,0 \end{cases}$$

4. $m$
   
   $$(4) \begin{cases} m & 0,y,z \\ (m_z) & 0,0,0 \end{cases}$$

For $(1/2,1/2,0)' + \text{ set}$

1. $t'$
   
   $$(1) \begin{cases} t' & (1/2,1/2,0) \\ (1') & (1/2,1/2,0) \end{cases}$$

2. $2'$
   
   $$(2) \begin{cases} 2' & 1/4,1/4,z \\ (2_{z'}) & 1/2,1/2,0' \end{cases}$$

3. $a'$
   
   $$(3) \begin{cases} a' & (1/2,0,0) \\ (a_y) & x,1/4,z \end{cases}$$

4. $b'$
   
   $$(4) \begin{cases} b' & (0,1/2,0) \\ (b_y) & 1/4,y,z \end{cases}$$
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry. Coordinates

(0,0,0) + (1/2,1/2,0)'

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 d .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>2 b mm2</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 a mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c_p mm2
a^* = a  b^* = b
Origin at 0,0,z

Along [1,0,0]  p1m11'
a^* = b/2  b^* = c
Origin at x,0,0

Along [0,1,0]  p1m11'
a^* = -a/2  b^* = c
Origin at 0,y,0
Asymmetric unit  \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) \quad & 1 \\
(2) \quad & 2 \quad 0,0,z \\
(3) \quad & m \quad x,0,z \\
(4) \quad & m \quad 0,y,z
\end{align*}
\]

\[
\begin{align*}
(1) \quad & 0,0,0 \\
(2) \quad & 0,0,0 \\
(3) \quad & 0,0,0 \\
(4) \quad & 0,0,0
\end{align*}
\]

For \((1/2,1/2,0) + \) set

\[
\begin{align*}
(1) \quad & t' \quad (1/2,1/2,0) \\
(2) \quad & 2' \quad 1/4,1/4,z \\
(3) \quad & a' \quad (1/2,0,0) \\
(4) \quad & b' \quad (0,1/2,0)
\end{align*}
\]

\[
\begin{align*}
(1) \quad & (1/2,1/2,0) \\
(2) \quad & (1/2,1/2,0) \\
(3) \quad & (1/2,1/2,0) \\
(4) \quad & (1/2,1/2,0)
\end{align*}
\]

For \((0,0,1) + \) set

\[
\begin{align*}
(1) \quad & t' \quad (0,0,1) \\
(2) \quad & 2' \quad (0,0,1) \\
(3) \quad & c' \quad (0,0,1) \\
(4) \quad & c' \quad (0,0,1)
\end{align*}
\]

\[
\begin{align*}
(1) \quad & (0,0,1) \\
(2) \quad & (0,0,1) \\
(3) \quad & (0,0,1) \\
(4) \quad & (0,0,1)
\end{align*}
\]

For \((1/2,1/2,1) + \) set

\[
\begin{align*}
(1) \quad & t \quad (1/2,1/2,1) \\
(2) \quad & 2 \quad (0,0,1) \\
(3) \quad & n \quad (1/2,0,1) \\
(4) \quad & n \quad (0,1/2,1)
\end{align*}
\]

\[
\begin{align*}
(1) \quad & (1/2,1/2,1) \\
(2) \quad & (1/2,1/2,1) \\
(3) \quad & (1/2,1/2,1) \\
(4) \quad & (1/2,1/2,1)
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>16 f</td>
<td>1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>m..</td>
<td>0,y,z [u,0,0] 0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 d</td>
<td>.m.</td>
<td>x,0,z [0,v,0] 0,v,0 [0,v,0]</td>
</tr>
<tr>
<td>8 c</td>
<td>.2'</td>
<td>1/4,1/4,z [u,v,0] 1/4,3/4,z [u,v,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>mm2</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2mm1'  Along [1,0,0]  p1m11'  Along [0,1,0]  p1m11'

a* = a  b* = b  a* = b/2  b* = c  a* = -a/2  b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Asymmetric unit  $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) + \text{set}$

(1) $1$
(2) $2' \quad 0,0,z$
(3) $m \quad x,0,z$
(4) $m' \quad 0,y,z$

For $(1/2,1/2,0) + \text{set}$

(1) $t \quad (1/2,1/2,0)$
(2) $2' \quad 1/4,1/4,z$
(3) $a \quad (1/2,0,0) \quad x,1/4,z$
(4) $b' \quad (0,1/2,0) \quad 1/4,y,z$

For $(0,0,1)' + \text{set}$

(1) $t' \quad (0,0,1)$
(2) $2 \quad (0,0,1) \quad 0,0,z$
(3) $c' \quad (0,0,1) \quad x,0,z$
(4) $c \quad (0,0,1) \quad 0,y,z$

For $(1/2,1/2,1)' + \text{set}$

(1) $t' \quad (1/2,1/2,1)$
(2) $2 \quad (0,0,1) \quad 1/4,1/4,z$
(3) $n' \quad (1/2,0,1) \quad x,1/4,z$
(4) $n \quad (0,1/2,1) \quad 1/4,y,z$
Continued

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

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<td>1</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>8 e</td>
<td>m'</td>
<td>0, y, z [0, v, w]</td>
</tr>
<tr>
<td>8 d</td>
<td>.m</td>
<td>x, 0, z [0, v, 0]</td>
</tr>
<tr>
<td>8 c</td>
<td>.2'</td>
<td>1/4, 1/4, z [u, v, 0]</td>
</tr>
<tr>
<td>4 b</td>
<td>m'm2'</td>
<td>0, 1/2, z [0, v, 0]</td>
</tr>
<tr>
<td>4 a</td>
<td>m'm2'</td>
<td>0, 0, z [0, v, 0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] c2mm1'
  - $a^* = a$, $b^* = b$
  - Origin at 0,0,z

- Along [1,0,0] p2b*1m1
  - $a^* = b/2$, $b^* = c$
  - Origin at x,0,0

- Along [0,1,0] p1m11'
  - $a^* = -a/2$, $b^* = c$
  - Origin at 0,y,0
Origin on mm'2

Asymmetric unit \(0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1\)

Symmetry Operations

For \((0,0,0) + \) set

1. \((0,0,0)\)
2. \(0,0,z\)
3. \(m'x,0,z\)
4. \(m'y,0,0)'^{'}\)

For \((1/2,1/2,0) + \) set

1. \(1/2,1/2,0)\)
2. \(1/2,1/4,1/4,z\)
3. \(a'(1/2,0,0)x,1/4,z\)
4. \(b'(0,1/2,0)1/4,y,z\)

For \((0,0,1)'+ \) set

1. \(0,0,1)\)
2. \(0,0,1)'\)
3. \(c(0,0,1)x,0,z\)
4. \(c(0,0,1)0,y,z\)

For \((1/2,1/2,1)'+ \) set

1. \(1/2,1/2,1)\)
2. \(1/2,1/4,1/4,z\)
3. \(n(1/2,0,1)x,1/4,z\)
4. \(n(0,1/2,1)1/4,y,z\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1'); t(1/2,1/2,0); (2); (3).

Positions

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<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,1') + (1/2,1/2,1')</td>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,1') + (1/2,1/2,1')</td>
</tr>
<tr>
<td>16 f 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e m'.. 0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 d .m' x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>8 c ..2 1/4,1/4,z [0,0,w]</td>
<td>1/4,3/4,z [0,0,w]</td>
</tr>
<tr>
<td>4 b  m'm'2 0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a  m'm'2 0,0,z [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
<th>Along [1,0,0]</th>
<th>p2b1m'1</th>
<th>Along [0,1,0]</th>
<th>p2b1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td></td>
<td>a* = b/2</td>
<td></td>
<td>a* = -a/2</td>
<td></td>
</tr>
<tr>
<td>b* = b</td>
<td></td>
<td>b* = c</td>
<td></td>
<td>b* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on m'm2'

Asymmetric unit
\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For (0,0,0) + set

1. \( \begin{align*} (1) \quad & \begin{cases} 1 \\ (1) 0,0,0 \end{cases} \\ (2') \quad & \begin{cases} 0,0,z \\ (2_z) 0,0,0' \end{cases} \\ (3) \quad & \begin{cases} m \quad & x,0,z \\ (m_y) \quad & 0,y,z \end{cases} \\ (4') \quad & \begin{cases} m' \quad & 0,y,z \\ (m_x) \quad & 0,0,0' \end{cases} \end{cases} \end{align*} \]

For \((1/2,1/2,0)\)' + set

1. \( \begin{align*} (1') \quad & \begin{cases} t' \quad & (1/2,1/2,0) \\ (1) \quad & (1/2,1/2,0)' \end{cases} \\ (2) \quad & \begin{cases} 2 \quad & 1/4,1/4,z \\ (2_z) \quad & 1/2,1/2,0 \end{cases} \\ (3) \quad & \begin{cases} a' \quad & (1/2,0,0) \\ (m_y) \quad & 1/2,1/2,0' \end{cases} \\ (4) \quad & \begin{cases} b \quad & 0,1/2,0 \\ (m_x) \quad & 1/2,1/2,0 \end{cases} \end{cases} \end{align*} \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)*; (2); (3).

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<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m'</td>
<td>0</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 d m'</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 c m'2'</td>
<td>1/4,1/4,z [0,0,w]</td>
<td>1/4,3/4,z [0,0,w]</td>
</tr>
<tr>
<td>2 b m'2'</td>
<td>0,1/2,z [0,v,0]</td>
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<tr>
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<td>0,0,z [0,v,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>c_p*2'mm'</td>
<td>p_2a*1m1</td>
<td>p1m11'</td>
</tr>
<tr>
<td>b* = a</td>
<td>a* = b/2</td>
<td>a* = -a/2</td>
<td>a* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on m'm'2

Asymmetric unit \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\) \((0,0,0)\)
2. \(2\) \((0,0,z)\)
3. \(m'\) \((x,0,z)\)
4. \(m'\) \((0,y,z)\)

For \((1/2,1/2,0)' + \) set

1. \(t'\) \((1/2,1/2,0)\)
2. \(2'\) \((1/4,1/4,z)\)
3. \(a\) \((1/2,0,0)\)
4. \(b\) \((0,1/2,0)\)

\((0,0,0)'\)
\((1/2,1/2,0)'\)
\((1/2,1/2,0)'\)
\((1/2,1/2,0)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

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<td>(0,0,0) + (1/2,1/2,0)' +</td>
<td></td>
</tr>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m'0</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 d m'1</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>4 c m'1</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>2 b m'12</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a m'12</td>
<td>0,0,z [0,0,w]</td>
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</tbody>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c_p2m'2m'</th>
<th>Along [1,0,0]</th>
<th>p_{2a1}m'1</th>
<th>Along [0,1,0]</th>
<th>p_{2a1}m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a b' = b</td>
<td>a' = b/2 b' = c</td>
<td>a' = -a/2 b' = c</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 1/4,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Asymmetric unit \[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1 \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1\)
2. \(2': 0,0,z\)
3. \(m\): \(x,0,z\)
4. \(m': 0,y,z\)

For \((1/2,1/2,0)'\) + set

1. \(t'\): \((1/2,1/2,0)\)
2. \(2: 1/4,1/4,z\)
3. \(a'(1/2,0,0): x,1/4,z\)
4. \(b: (0,1/2,0): 1/4,y,z\)

For \((0,0,1)\) + set

1. \(t'\): \((0,0,1)\)
2. \(2: 0,0,1\)
3. \(c'(0,0,1): x,0,z\)
4. \(c: (0,0,1): 0,y,z\)

For \((1/2,1/2,1)\) + set

1. \(t\): \((1/2,1/2,1)\)
2. \(2': (0,0,1)\)
3. \(n(1/2,0,1): x,1/4,z\)
4. \(n': (0,1/2,1): 1/4,y,z\)
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e m</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 d m</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 c m</td>
<td>1/4,1/4,z [0,0,w]</td>
<td>1/4,3/4,z [0,0,w]</td>
</tr>
<tr>
<td>4 b m</td>
<td>0,1/2,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 a m</td>
<td>0,0,z [0,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c2mm1'</th>
<th>Along [1,0,0] p1m1'</th>
<th>Along [0,1,0] p1m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a b' = b</td>
<td>a' = b/2 b' = c</td>
<td>a' = -a/2 b' = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
CI m’m'2
35.13.248
C m’m'2

Origin on m’m'2

Asymmetric unit

0 < x < 1/4; 0 < y < 1/2; 0 < z < 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z
(3) m' x,0,z
(4) m' 0,y,z

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(2) 2' 1/4,1/4,z
(3) a (1/2,0,0) x,1/4,z
(4) b (0,1/2,0) 1/4,y,z

For (0,0,1)' + set

(1) t' (0,0,1)
(2) 2' (0,0,1) 0,0,z
(3) c (0,0,1) x,0,z
(4) c (0,0,1) 0,y,z

For (1/2,1/2,1) + set

(1) t (1/2,1/2,1)
(2) 2 (0,0,1) 1/4,1/4,z
(3) n' (1/2,0,1) x,1/4,z
(4) n' (0,1/2,1) 1/4,y,z

35.13.248 - 1 - 472
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity,</td>
<td></td>
</tr>
<tr>
<td>Wyckoff letter,</td>
<td></td>
</tr>
<tr>
<td>Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>(0,0,0) + (1/2,1/2,0) +</td>
<td>(1/2,1/2,1) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>(0,0,1) + (1/2,1/2,1) +</td>
<td></td>
</tr>
<tr>
<td>16 f 1 (1) x,y,z [u,v,w]</td>
<td>(2) x̅,y̅,z [u̅,v̅,w] (3) x̅,y̅,z [u̅,v̅,w] (4) x̅,y̅,z [u̅,v̅,w]</td>
</tr>
<tr>
<td>8 e m'.. 0,y,z [0,v,w]</td>
<td>0,y,z [0,v̅,w]</td>
</tr>
<tr>
<td>8 d .m'.. x,0,z [u,0,w]</td>
<td>x̅,0,z [u̅,0,w]</td>
</tr>
<tr>
<td>8 c .2' 1/4,1/4,z [u,v,0]</td>
<td>1/4,3/4,z [u̅,v̅,0]</td>
</tr>
<tr>
<td>4 b m'm'2 0,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 a m'm'2 0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c2mm1'</th>
<th>Along [1,0,0] p_c1m1</th>
<th>Along [0,1,0] p_c1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a   b* = b</td>
<td>a* = b/2 b* = c</td>
<td>a* = -a/2 b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 1/4,y,0</td>
</tr>
</tbody>
</table>
36.1.249 - Cmc2₁ Orthorhombic

Origin on mc2₁

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

1. $1$
2. $0,0,0$
3. $0,0,1/2$
4. $x,0,z$
5. $c (0,0,1/2)$
6. $0,y,z$

For (1/2,1/2,0) + set

1. $t (1/2,1/2,0)$
2. $0,0,1/2$
3. $1/4,1/4,z$
4. $x,1/4,z$
5. $n (1/2,0,1/2)$
6. $1/4,y,z$
7. $x,1/4,z$
8. $m (0,0,0)$
9. $0,y,z$
10. $x,1/4,z$
11. $m (0,0,1/2)$
12. $1/4,y,z$
13. $x,1/4,z$
14. $m (0,1/2,0)$
15. $1/4,y,z$
16. $x,1/4,z$
17. $m (1/2,1/2,0)$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 a m..</td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2mm
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0]  p1g11*
a* = b/2  b* = c
Origin at x,0,0

Along [0,1,0]  p2v,1m1
a* = -a/2  b* = c/2
Origin at 0,y,0
Cmc2\textsubscript{1}'

36.2.250

\begin{align*}
\text{Origin} & \quad \text{on mc2,1}' \\
\text{Asymmetric unit} & \quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2
\end{align*}

Symmetry Operations

\begin{align*}
\text{For } (0,0,0) + \text{ set} & \\
(1) & \quad 1 \\
(2) & \quad \begin{array}{c} (0,0,1/2) \\
(2_x,0,0,1/2) \end{array} \\
(3) & \quad \begin{array}{c} c (0,0,1/2) \\
(m_y,0,0,1/2) \end{array} \\
(4) & \quad \begin{array}{c} m \quad 0,y,z \\
(m_x,0,0,0) \end{array}
\end{align*}

\begin{align*}
\text{For } (1/2,1/2,0) + \text{ set} & \\
(1) & \quad t (1/2,1/2,0) \\
(2) & \quad \begin{array}{c} (0,0,1/2) \\
(2_x,1/2,1/2,1/2) \end{array} \\
(3) & \quad \begin{array}{c} n (1/2,0,1/2) \\
(m_y,1/2,1/2,1/2) \end{array} \\
(4) & \quad \begin{array}{c} b (0,1/2,0) \\
(m_x,1/2,1/2,0) \end{array}
\end{align*}

\begin{align*}
\text{For } (0,0,0)' + \text{ set} & \\
(1) & \quad 1' \\
(2) & \quad \begin{array}{c} (0,0,1/2) \\
(2_x,0,0,1/2') \end{array} \\
(3) & \quad \begin{array}{c} c' (0,0,1/2) \\
(m_y,0,0,1/2') \end{array} \\
(4) & \quad \begin{array}{c} m' \quad 0,y,z \\
(m_x,0,0,0)' \end{array}
\end{align*}

\begin{align*}
\text{For } (1/2,1/2,0)' + \text{ set} & \\
(1) & \quad t' (1/2,1/2,0) \\
(2) & \quad \begin{array}{c} (0,0,1/2) \\
(2_x,1/2,1/2,1/2') \end{array} \\
(3) & \quad \begin{array}{c} n' (1/2,0,1/2) \\
(m_y,1/2,1/2,1/2') \end{array} \\
(4) & \quad \begin{array}{c} b' (0,1/2,0) \\
(m_x,1/2,1/2,0)' \end{array}
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a m..1'</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1'  Along [1,0,0] p1g11'  Along [0,1,0] p1m11'

\(a^* = a\)  \(b^* = b\)  \(a^* = b/2\)  \(b^* = c\)  \(a^* = -a/2\)  \(b^* = c/2\)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
**Orthorhombic**

36.3.251

Cm'c2ι

m'm2'

**Origin** on m'c2ι

**Asymmetric unit**

\[0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2\]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \(1\)
2. \(2' (0,0,1/2) \quad 0,0,z\)
3. \(c (0,0,1/2) \quad x,0,z\)
4. \(m' \quad 0,y,z\)

\(\text{For } (1/2,1/2,0) + \text{set}\)

1. \(t (1/2,1/2,0) \quad 1/2,1/2,1/2'\)
2. \(2' (0,0,1/2) \quad 1/4,1/4,z\)
3. \(n (1/2,0,1/2) \quad x,1/4,z\)
4. \(b' (0,1/2,0) \quad 1/4,y,z\)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w] (2) x̅,y,z+1/2 [u,v,w] (3) x̅,y,z+1/2 [u,v,w] (4) x̅,y,z [u̅,v,w]</td>
</tr>
<tr>
<td>4 a m'..</td>
<td>0,y,z [0,v,w] 0,y̅,z+1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm' Along [1,0,0] p1g1 Along [0,1,0] p21m1

a* = -b  b* = a a* = b/2  b* = c a* = -a/2  b* = c/2

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin on mc’2₁⁺

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \]

Symmetry Operations

For (0,0,0) + set

(1) \( \mathbf{i} \) \hspace{1cm} (2) \( \mathbf{2'} \) \hspace{1cm} (3) \( \mathbf{c'} \) \hspace{1cm} (4) \( \mathbf{m} \)

\[ (1|0,0,0) \rightarrow (2|0,0,1/2) \rightarrow (3|0,0,1/2) \rightarrow (4|0,0,0) \]

For (1/2,1/2,0) + set

(1) \( \mathbf{t} \) \hspace{1cm} (2) \( \mathbf{2'} \) \hspace{1cm} (3) \( \mathbf{n'} \) \hspace{1cm} (4) \( \mathbf{b} \)

\[ (1|1/2,1/2,0) \rightarrow (2|0,0,1/2) \rightarrow (3|1/2,0,1/2) \rightarrow (4|0,1/2,0) \]
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

<table>
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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 a m..</td>
<td>0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  c2mm$'$     
Along [1,0,0]  p1g11$'$     
Along [0,1,0]  p1m1

\[a^* = a \quad b^* = b\] 
\[a^* = b/2 \quad b^* = c\] 
\[a^* = -a/2 \quad b^* = c/2\]

Origin at 0,0,z 
Origin at x,0,0 
Origin at 0,y,0
Symmetry Operations

For $(0,0,0) + \text{ set}$

(1) $1$  
(2) $2 (0,0,1/2) \quad 0,0,z$  
(3) $c' (0,0,1/2) \quad x,0,z$  
(4) $m' \quad 0,y,z$  

For $(1/2,1/2,0) + \text{ set}$

(1) $t (1/2,1/2,0)$  
(2) $2 (0,0,1/2) \quad 1/4,1/4,z$  
(3) $n' (1/2,0,1/2) \quad x,1/4,z$  
(4) $b' (0,1/2,0) \quad 1/4,y,z$  

Origin on $m'c'2_1$  

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

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<tr>
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<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) +</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 b 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 a m' 0,y,z [0,v,w]</td>
<td>0,y,z+1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2m'm'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0] p1g'1  
\( \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [0,1,0] p1m'1  
\( \mathbf{a}^* = -\mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at 0,y,0
**Origin** on mc$_2_1$

**Asymmetric unit**  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

1. $1$
2. $(2)$ (0,0,1/2) 0,0,z
3. $c$ (0,0,1/2) x,0,z
4. $m$ 0,y,z
5. $(m_1,0,0,0)$

For (1/2,1/2,0) + set

1. $t'$ (1/2,1/2,0) 0,0,1/4
2. $(2')$ (0,0,1/2) 1/4,1/4,z
3. $n'$ (1/2,0,1/2) x,1/4,z
4. $b'$ (0,1/2,0) 1/4,y,z
5. $(m_1,0,0,0)$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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</tr>
<tr>
<td>4 a m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_p,2mm

a* = a  b* = b

Origin at 0,0,z
Origin on m'c2₁⁺

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z
(2|0,0,1/2)⁺

(3) c (0,0,1/2) x,0,z
(m₁|0,0,1/2)

(4) m' 0,y,z
(m₂|0,0,0)⁺

For (1/2,1/2,0)⁺ + set

(1) t' (1/2,1/2,0)
(1|1/2,1/2,0)⁺

(2) 2 (0,0,1/2) 1/4,1/4,z
(2|1/2,1/2,1/2)

(3) n' (1/2,0,1/2) x,1/4,z
(m₃|1/2,1/2,1/2)⁺

(4) b (0,1/2,0) 1/4,y,z
(m₄|1/2,1/2,0)⁺
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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</tr>
<tr>
<td></td>
<td>(2) x',y',z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y',z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 d' m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y',z+1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( \text{c}_p\cdot 2\text{mm}' \) Along [1,0,0] \( \text{p}_{2a}\cdot 1\text{g1} \) Along [0,1,0] \( \text{p}_c\cdot 1\text{m1} \)

\( \mathbf{a}^* = -\mathbf{b} \quad \mathbf{b}^* = \mathbf{a} \) \quad \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c} \) \quad \mathbf{a}^* = -\mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{c}/2 

Origin at 0,0,z \quad \text{Origin at } x,0,0 \quad \text{Origin at } 1/4,y,0
C\textsubscript{p}mc'2\textsubscript{1},'  
mm21'  
Orthorhombic  
36.8.256  
C\textsubscript{p}mc'2\textsubscript{1},'

**Origin**  on mc'2\textsubscript{1},'

**Asymmetric unit**  
0 \leq x \leq 1/2;  
0 \leq y \leq 1/2;  
0 \leq z \leq 1/2

**Symmetry Operations**

For (0,0,0) + set

(1) 1
(2) 2' (0,0,1/2) 0,0,z
(3) c' (0,0,1/2) x,0,z
(4) m 0,y,z

(1*) 0,0,0
(2* 0,0,1/2)
(3* m,0,0,1/2')
(4* m,0,0,0)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(2) 2 (0,0,1/2) 1/4,1/4,z
(3) n (1/2,0,1/2) x,1/4,z
(4) b' (0,1/2,0) 1/4,y,z

(1') 1/2,1/2,0
(2' 1/2,1/2,1/2)
(3' m,1/2,1/2,1/2)
(4' m,1/2,1/2,0)'

36.8.256 - 1 - 488
Continued

Generators selected

(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[(0,0,0) + \frac{1}{2}(1,1,0)\]

8 b 1 (1) x,y,z [u,v,w] (2) x,y,z+1/2 [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w]

4 a m. 0,y,z [u,0,0] 0,y,z+1/2 [u,0,0]

Symmetry of Special Projections

\[\begin{align*}
\text{Along } [0,0,1] & \quad c_{p,2'mm}' \\
\text{Along } [1,0,0] & \quad p1g11' \\
\text{Along } [0,1,0] & \quad p_{2z,1m1}
\end{align*}\]

\[\begin{align*}
\mathbf{a}^* = \mathbf{a} & \quad \mathbf{b}^* = \mathbf{b} \\
\mathbf{a}^* = \mathbf{b}/2 & \quad \mathbf{b}^* = \mathbf{c} \\
\mathbf{a}^* = -\mathbf{a}/2 & \quad \mathbf{b}^* = \mathbf{c}/2
\end{align*}\]

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin on m’c’2₁

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1  
(2) ₂ (0,0,1/2)  0,0,z  
(3) c’ (0,0,1/2) x,0,z  
(4) m’ 0,y,z  

For (1/2,1/2,0)’ + set

(1) t’ (1/2,1/2,0)  
(2) ₂’ (0,0,1/2)  1/4,1/4,z  
(3) n (1/2,0,1/2) x,1/4,z  
(4) b (0,1/2,0)  1/4,y,z  

\[ C_p m’c’2₁ \quad mm2₁’ \quad Orthorhombic \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
(0,0,0) &\quad + & (1/2,1/2,0)' &\quad + \\
8 &\quad b &\quad 1 &\quad (1) \ x,y,z \ [u,v,w] &\quad (2) \ \bar{x},\bar{y},z+1/2 \ [\bar{u},\bar{v},w] &\quad (3) \ x,\bar{y},z+1/2 \ [u,\bar{v},w] &\quad (4) \ \bar{x},y,z \ [\bar{u},v,w] \\
4 &\quad a &\quad m' &\quad 0,y,z \ [0,v,w] &\quad 0,\bar{y},z+1/2 \ [0,\bar{v},w]
\end{align*}
\]

Symmetry of Special Projections

Along [0,0,1] \ {c_p, 2m'm'} \quad Along [1,0,0] \ p_{2a'1g1} \quad Along [0,1,0] \ p_{2a'1m1}

\[
\begin{align*}
a^* &= a &\quad b^* &= b \\
a^* &= b/2 &\quad b^* &= c &\quad a^* &= -a/2 &\quad b^* &= c/2
\end{align*}
\]

Origin at 0,0,z \quad Origin at x,1/4,0 \quad Origin at 1/4,y,0
Origin on cc2

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

1 (0,0,0) (2) 0,0,z (3) c (0,0,1/2) x,0,z (4) c (0,0,1/2) 0,y,z
(1) (2,0,0) (2,1/4,0,0) (m,0,0,1/2) (m,0,0,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (2) 1/4,1/4,z (3) n (1/2,0,1/2) x,1/4,z (4) n (0,1/2,1/2) 1/4,y,z
(1) (2,1/2,1/2,0) (2,1/2,1/2,0) (m,1/2,1/2,1/2) (m,1/2,1/2,1/2)
Generators selected  (1); t(1,0,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 d 1</td>
<td>(1) (x, y, z \ [u, v, w])</td>
</tr>
<tr>
<td></td>
<td>(2) (\bar{x}, \bar{y}, \bar{z} \ [\bar{u}, \bar{v}, \bar{w}])</td>
</tr>
<tr>
<td></td>
<td>(3) (x, y, z+1/2 \ [u, v, w])</td>
</tr>
<tr>
<td></td>
<td>(4) (\bar{x}, \bar{y}, \bar{z}+1/2 \ [\bar{u}, \bar{v}, \bar{w}])</td>
</tr>
<tr>
<td>4 c .2</td>
<td>1/4,1/4,0 (0,0,0)</td>
</tr>
<tr>
<td></td>
<td>1/4,3/4,z+1/2 (0,0,0)</td>
</tr>
<tr>
<td>4 b .2</td>
<td>0,1/2,z (0,0,0)</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 (0,0,0)</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,0 (0,0,0)</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 (0,0,0)</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\)  c2mm
  - \(\mathbf{a}^* = \mathbf{b}\)
  - \(\mathbf{b}^* = \mathbf{b}\)
- Along \([1,0,0]\)  \(p2\_1m'1\)
  - \(\mathbf{a}^* = \mathbf{b}/2\)
  - \(\mathbf{b}^* = \mathbf{c}/2\)
- Along \([0,1,0]\)  \(p2\_1m'1\)
  - \(\mathbf{a}^* = -\mathbf{a}/2\)
  - \(\mathbf{b}^* = \mathbf{c}/2\)

Origin at 0,0,0
Origin at \(x,0,0\)
Origin at 0,y,0
**Origin** on cc21'

**Asymmetric unit**  
\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1 (0,0,0)\)
2. \(2 \quad 0,0,z\)
3. \(c (0,0,1/2)\)
4. \(c (0,0,1/2)\)

For \((1/2,1/2,0)\) + set

1. \(t (1/2,1/2,0)\)
2. \(2 \quad 1/4,1/4,z\)
3. \(n (1/2,0,1/2)\)
4. \(n (0,1/2,1/2)\)

For \((0,0,0)\)' + set

1. \(1' (0,0,0)\)
2. \(2' \quad 0,0,z\)
3. \(c' (0,0,1/2)\)
4. \(c' (0,0,1/2)\)

For \((1/2,1/2,0)\)' + set

1. \(t' (1/2,1/2,0)\)
2. \(2' \quad 1/4,1/4,z\)
3. \(n' (1/2,0,1/2)\)
4. \(n' (0,1/2,1/2)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>(0,0,0) + (1/2,1/2,0) + (0,0,0)' + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>4</td>
<td>x,y,z [0,0,0] (2) x,y,z+1/2 [0,0,0] (3) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>1/4,1/4,z [0,0,0] 1/4,3/4,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>0,1/2,z [0,0,0] 0,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>0,0,z [0,0,0] 0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1'  Along [1,0,0] p1m11'  Along [0,1,0] p1m11'

a* = a  b* = b  a* = b/2  b* = c/2  a* = -a/2  b* = c/2
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on $c'c2'$

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) + \text{ set}$

1. $1$
   
2. $2' \quad 0,0,z$
   
3. $c \quad (0,0,1/2) \quad x,0,z$
   
4. $c' \quad (0,0,1/2) \quad 0,y,z$

For $(1/2,1/2,0) + \text{ set}$

1. $t \quad (1/2,1/2,0)$
   
2. $2' \quad 1/4,1/4,z$
   
3. $n \quad (1/2,0,1/2) \quad x,1/4,z$
   
4. $n' \quad (0,1/2,1/2) \quad 1/4,y,z$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,0)</td>
</tr>
</tbody>
</table>

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0) +</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>d</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) x,y,z+1/2 [u,v,w]</th>
<th>(4) x,y,z+1/2 [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>c</td>
<td>.2'</td>
<td>1/4,1/4,z [u,v,0]</td>
<td>1/4,3/4,z+1/2 [u,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>.2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>0,1/2,z+1/2 [u,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>.2'</td>
<td>0,0,z [u,v,0]</td>
<td>0,0,z+1/2 [u,v,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm'</th>
<th>Along [1,0,0]</th>
<th>p1m1</th>
<th>Along [0,1,0]</th>
<th>p2v,1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a</td>
<td>a* = b/2</td>
<td>b* = c/2</td>
<td>a* = -a/2</td>
<td>b* = c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Asymmetric unit \[0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\]

Symmetry Operations

For \((0,0,0) + \text{ set}\)

1. \((1)\) 1
2. \((2)\) 2, 0,0, z
3. \((3)\) c' (0,0,1/2), x,0,z
4. \((4)\) c' (0,0,1/2), 0,y,z

\( (m_y, 0, 0, 1/2)' \)

\( (m_z, 0, 0, 1/2)' \)

For \((1/2,1/2,0) + \text{ set}\)

1. \((1)\) t (1/2,1/2,0)
2. \((2)\) 2, 1/4,1/4, z
3. \((3)\) n' (1/2,0,1/2), x,1/4,z
4. \((4)\) n' (0,1/2,1/2), 1/4,y,z

\( (m_y, 1/2, 1/2, 1/2)' \)

\( (m_z, 1/2, 1/2, 1/2)' \)
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3). \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) ( x, y, z [\bar{u},\bar{v},w] )</td>
</tr>
<tr>
<td>4 c .2</td>
<td>1/4,1/4,z [0,0,w]</td>
<td>1/4,3/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 b .2</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along \([0,0,1]\)  \( \text{c2m' m'} \)
  - \( a^* = a \) \( b^* = b \)
  - Origin at 0,0,z

- Along \([1,0,0]\)  \( \text{p1m'1} \)
  - \( a^* = b/2 \) \( b^* = c/2 \)
  - Origin at x,0,0

- Along \([0,1,0]\)  \( \text{p1m'1} \)
  - \( a^* = -a/2 \) \( b^* = c/2 \)
  - Origin at 0,y,0
CPcc2  mm21'  Orthorhombic

37.5.262  C_Pcc2

Origin  on cc2

Asymmetric unit  0 ≤ x ≤ 1/4;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1)  1
(1 | 0,0,0)
(2)  2  0,0,z
(2z | 0,0,0)
(3)  c  (0,0,1/2)  x,0,z
(my | 0,0,1/2)
(4)  c  (0,0,1/2)  0,y,z
(mx | 0,0,1/2)

For (1/2,1/2,0)' + set

(1)  t'  (1/2,1/2,0)
(1 | 1/2,1/2,0)' (2)  2'  1/4,1/4,z
(2z | 1/2,1/2,0)'
(3)  n'  (1/2,0,1/2)  x,1/4,z
(my | 1/2,1/2,1/2)'
(4)  n'  (0,1/2,1/2)  1/4,y,z
(mx | 1/2,1/2,1/2)'
Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0)'; (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>4 b .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] cₚ₂mm  
Along [1,0,0] pₐ₁m₁  
Along [0,1,0] pₚ₁m₁

a* = a  b* = b  
a* = b/2  b* = c/2  
a* = -a/2  b* = c/2  

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at 1/4,y,0
Origin on c'c2'

Asymmetric unit \(0 \leq x \leq 1/4;\) \(0 \leq y \leq 1/2;\) \(0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0)+\) set

1. \(1\)
2. \((2') (0,0,0)\) \((2,0,0)\) \((1,0,0)\)
3. \((c) (0,0,1/2) x,0,z\) \((m,0,0,1/2)\)
4. \((c') (0,0,1/2) 0,y,z\) \((m,0,0,1/2)\)

For \((1/2,1/2,0)^{+}\) set

1. \(t' (1/2,1/2,0)\)
2. \((2) 1/4,1/4,z\) \((2,1/2,0)\) \((1,1/2,0)\)
3. \((n') (1/2,0,1/2) x,1/4,z\) \((m,1/2,1/2,0)\)
4. \((n) (0,1/2,1/2) 1/4,y,z\) \((m,1/2,1/2,0)\)
Generators selected  (1); t(1,0,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) (\overline{x},\overline{y},\overline{z} [u,v,w])</td>
</tr>
<tr>
<td></td>
<td>(3) x,(\overline{y},\overline{z}+1/2 [u,v,w])</td>
</tr>
<tr>
<td></td>
<td>(4) (\overline{x},y,z+1/2 [u,v,w])</td>
</tr>
<tr>
<td>4 c ..2</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,3/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 b ..2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \(c_p2'\text{mm}'\) \(a^* = -b\quad b^* = a\) \(\text{Origin at } 0,0,z\)
Along [1,0,0] \(p_{2a1m1}\) \(a^* = b/2\quad b^* = c/2\) \(\text{Origin at } x,0,0\)
Along [0,1,0] \(p_{2a1m1}\) \(a^* = -a/2\quad b^* = c/2\) \(\text{Origin at } 0,y,0\)
Asymmetric unit: $0 \leq x \leq 1/4$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set:

(1) $1$
(2) $2$, $0,0,z$
(3) $c'$ $(0,0,1/2)$, $x,0,z$
(4) $c'$ $(0,0,1/2)$, $0,y,z$

(1*) $(1/2,1/2,0)$
(2*) $1/4,1/4,z$
(3*) $n$ $(1/2,0,1/2)$, $x,1/4,z$
(4*) $n$ $(0,1/2,1/2)$, $1/4,y,z$

For $(1/2,1/2,0)'$ + set:

(1) $t'$ $(1/2,1/2,0)$
(2) $2'$ $1/4,1/4,z$
(3) $n$ $(1/2,0,1/2)$, $x,1/4,z$
(4) $n$ $(0,1/2,1/2)$, $1/4,y,z$

(1*) $(1/2,1/2,0)'$
(2*) $1/2,1/2,0'$
(3*) $(1/2,0,1/2)'$
(4*) $(0,1/2,1/2)'$

Symmetry Operations:

- $(1)\ 1$
- $(2)\ 2, 0,0,z$
- $(3)\ c' (0,0,1/2), x,0,z$
- $(4)\ c' (0,0,1/2), 0,y,z$

- $(1*)\ (1/2,1/2,0)$
- $(2*)\ 1/4,1/4,z$
- $(3*)\ n (1/2,0,1/2), x,1/4,z$
- $(4*)\ n (0,1/2,1/2), 1/4,y,z$

Origin: on $c'c'2$
Continued

Generators selected
(1); t(1,0,0); t(0,0,0); t(0,0,1); t(1/2,1/2,0); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>x, y, z [u, v, w]</td>
<td>(0,0,0) + (1/2, 1/2, 0)' + (0,0,0) + (1/2, 1/2, 0)' +</td>
<td>(2) x, y, z [u, v, w] (3) x, y, z+1/2 [u, v, w] (4) x, y, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td>4 c 2'</td>
<td>1/4, 1/4, z [u, v, 0]</td>
<td>1/4, 3/4, z+1/2 [u, v, w]</td>
<td>1/4, 1/4, z [u, v, 0]</td>
</tr>
<tr>
<td>4 b 2</td>
<td>1/2, z [0, 0, w]</td>
<td>0, 1/2, z+1/2 [0, 0, w]</td>
<td>0, 1/2, z [0, 0, w]</td>
</tr>
<tr>
<td>4 a 2</td>
<td>0, 0, z [0, 0, w]</td>
<td>0, 0, z+1/2 [0, 0, w]</td>
<td>0, 0, z [0, 0, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0, 0, 1] c_p 2m’m’  Origin at 0, 0, z
a* = a  b* = b

Along [1, 0, 0] p_2a 1m’1  Origin at x, 0, 0
a* = b/2  b* = c/2

Along [0, 1, 0] p_2a 1m’1  Origin at 0, y, 0
a* = -a/2  b* = c/2
### Amm2 in mm2

**Origin** on mm2

**Asymmetric unit**

\[
0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}
\]

**Symmetry Operations**

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 0,0,z \\
(3) & \quad m,0,0 \\
(4) & \quad 0,y,z
\end{align*}
\]

For \((0,1/2,1/2) + \) set

\[
\begin{align*}
(1) & \quad t,0,1/2 \\
(2) & \quad 2,0,1/2 \\
(3) & \quad c,0,1/2 \\
(4) & \quad n,0,1/2
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

(0,0,0) + (0,1/2,1/2) +

8 f 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]
4 e m.. 1/2,y,z [u,0,0] 1/2,y,z [u,0,0]
4 d m.. 0,y,z [u,0,0] 0,y,z [u,0,0]
4 c .m. x,0,z [0,v,0] x,0,z [0,v,0]
2 b mm2 1/2,0,z [0,0,0]
2 a mm2 0,0,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2mm Along [1,0,0] c1m11' Along [0,1,0] p1m11'
\( a^* = a \) \( b^* = b/2 \) \( a^* = b \) \( b^* = c \) \( a^* = -a \) \( b^* = c/2 \)
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
**Origin** on mm21'

**Asymmetric unit**  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

1. $t (0,0,0) \rightarrow (1|0,0,0)$  
   (2) $2 (0,0,0) \rightarrow (0,0,z) \rightarrow (2|0,0,0)$  
   (3) $m (0,0,0) \rightarrow (x,0,z) \rightarrow (m|0,0,0)$  
   (4) $m (0,0,0) \rightarrow (0,y,z) \rightarrow (m|0,0,0)$

For (0,1/2,1/2) + set

1. $t (0,1/2,1/2) \rightarrow (1|0,1/2,1/2)$  
   (2) $2 (0,0,1/2) \rightarrow (0,0,z) \rightarrow (2|0,1/2,1/2)$  
   (3) $c (0,0,1/2) \rightarrow (0,0,z) \rightarrow (m|0,0,1/2)$  
   (4) $n (0,1/2,1/2) \rightarrow (0,0,z) \rightarrow (m|0,0,1/2)$

For (0,0,0)’ + set

1. $t (0,1/2,1/2) \rightarrow (1|0,1/2,1/2)$  
   (2) $2 (0,0,1/2) \rightarrow (0,0,z) \rightarrow (2|0,1/2,1/2)$  
   (3) $m (0,0,0) \rightarrow (0,0,z) \rightarrow (m|0,0,0)$  
   (4) $m (0,0,0) \rightarrow (0,y,z) \rightarrow (m|0,0,0)$

For (0,1/2,1/2)’ + set

1. $t (0,0,0) \rightarrow (1|0,1/2,1/2)$  
   (2) $2 (0,0,1/2) \rightarrow (0,0,z) \rightarrow (2|0,1/2,1/2)$  
   (3) $c (0,0,1/2) \rightarrow (0,0,z) \rightarrow (m|0,0,1/2)$  
   (4) $n (0,1/2,1/2) \rightarrow (0,0,z) \rightarrow (m|0,0,1/2)$
Generators selected  (1); t(1,0,0); t(0,0,1); t(0,1,0); t(0,1/2,1/2); (2); (3); 1'.

<table>
<thead>
<tr>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) +</td>
</tr>
<tr>
<td>(0,0,0)' + (0,1/2,1/2)' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 11'</td>
<td>1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3) x,y,z [0,0,0]</td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 e m..1'</td>
<td>1/2,y,z [0,0,0]</td>
<td>1/2,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 d m..1'</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 c .m.1'</td>
<td>x,0,z [0,0,0]</td>
<td>x,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 b mm21'</td>
<td>1/2,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a mm21'</td>
<td>0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2mm1'</th>
<th>Along [1,0,0] c1m11'</th>
<th>Along [0,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b/2</td>
<td>a* = b b* = c</td>
<td>a* = -a b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Am'm2' m'm2' Orthorhombic

38.3.267 Am'm2'

Origin on m'm2'

Asymmetric unit \(0 < x < \frac{1}{2}; 0 < y < \frac{1}{2}; 0 < z < \frac{1}{2}\)

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \((1) \quad 1\)
   
   \((1|0,0,0)\)

2. \((2) \quad 2' \quad 0,0,z\)
   
   \((2|0,0,0)\)

3. \((3) \quad m \quad x,0,z\)
   
   \((m|0,0,0)\)

4. \((4) \quad m' \quad 0,y,z\)
   
   \((m'|0,0,0)\)

For \((0,1/2,1/2) + \text{set}\)

1. \((1) \quad t\)
   
   \((1|0,1/2,1/2)\)

2. \((2) \quad 2' \quad (0,0,1/2) \quad 0,1/4,z\)
   
   \((2|0,1/2,1/2)\)

3. \((3) \quad c \quad (0,0,1/2) \quad x,1/4,z\)
   
   \((m|0,1/2,1/2)\)

4. \((4) \quad n' \quad (0,1/2,1/2) \quad 0,y,z\)
   
   \((m'_z,0,1/2,1/2)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m'..</td>
<td>1/2,y,z [0,v,w] 1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 d m'..</td>
<td>0,y,z [0,v,w] 0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,0,z [0,v,0] x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 b m'm2'</td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 a m'm2'</td>
<td>0,0,z [0,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p2'mmm'</td>
<td>c1m1</td>
<td>p1m11'</td>
</tr>
<tr>
<td>a* = -b/2</td>
<td>a* = b</td>
<td>a* = -a</td>
</tr>
<tr>
<td>b* = a</td>
<td>b* = c</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin on mm’2’

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2’ 0,0,z
(3) m’ x,0,z
(4) m 0,y,z

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)
(2) 2’ (0,0,1/2) 0,1/4,z
(3) c’ (0,0,1/2) x,1/4,z
(4) n (0,1/2,1/2) 0,y,z
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

#### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m..</td>
<td>1/2,y,z [u,0,0]</td>
<td>1/2,y,z [u,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 d m..</td>
<td>0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 c m'..</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b mm'2'</td>
<td>1/2,0,z [u,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a mm'2'</td>
<td>0,0,z [u,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Symmetry of Special Projections

Along [0,0,1] p2'nm'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}/2 \)

Along [1,0,0] c1m11'  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)

Along [0,1,0] p1m1  
\( \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2 \)

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Am'm'2  
38.5.269  
Orthorhombic  
m'm'2  
Am'm'2

Origin: on m'm'2

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) + \text{set}$

1. $1$  
   (1) $0,0,0$  
   (2) $0,0,z$  
   (3) $m', x,0,z$  
   (4) $m'_{0,y,z}$  
   (m$|0,0,0')$

For $(0,1/2,1/2) + \text{set}$

1. $t (0,1/2,1/2)$  
   (1) $0,1/2,1/2$  
   (2) $0,0,1/2$  
   (3) $c' (0,0,1/2)$  
   (4) $n' (0,1/2,1/2)$  
   (m$|0,1/2,1/2')$

   (2z$|0,0,0$)  
   (2z$|0,1/2,1/2$)  
   (m$|y,0,0$)  
   (m$|0,1/2,1/2')$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>8  f  1 (1) x,y,z [u,v,w]</td>
<td>(2) x̅,y̅,z [u̅,v̅,w]</td>
</tr>
<tr>
<td>4  e  m'.. 1/2,y,z [0,v,w]</td>
<td>1/2,y̅,z [0,v̅,w]</td>
</tr>
<tr>
<td>4  d  m'.. 0,y,z [0,v,w]</td>
<td>0,y̅,z [0,v̅,w]</td>
</tr>
<tr>
<td>4  c  m'.. x,0,z [u,0,w]</td>
<td>x̅,0,z [u̅,0,w]</td>
</tr>
<tr>
<td>2  b  m'm'2 1/2,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2  a  m'm'2 0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2m'm'</th>
<th>Along [1,0,0] c1m'1</th>
<th>Along [0,1,0] p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a    b' = b/2</td>
<td>a' = b    b' = c</td>
<td>a' = -a   b' = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin on mm2

Asymmetric unit $0 \leq x \leq 1/2;\quad 0 \leq y \leq 1/2;\quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $I (0,0,0)$
   
2. $2 (0,0,z)$
   
3. $m (x,0,z)$
   
4. $m (0,y,z)$

For $(0,1/2,1/2)$ + set

1. $t (0,1/2,1/2)$
   
2. $2 (0,0,1/2)\quad 0,1/4,z$
   
3. $c (0,0,1/2)\quad x,1/4,z$
   
4. $n (0,1/2,1/2)\quad 0,y,z$

For $(1,0,0')$ + set

1. $t (1,0,0)$
   
2. $2' (1/2,0,z)$
   
3. $a' (1,0,0)\quad x,0,z$
   
4. $m' (1/2,y,z)$

For $(1,1/2,1/2)$ + set

1. $t' (1,1/2,1/2)$
   
2. $2' (0,0,1/2)\quad 1/2,1/4,z$
   
3. $n' (1,0,1/2)\quad x,1/4,z$
   
4. $n' (0,1/2,1/2)\quad 1/2,y,z$

For $(0,1/2,1/2)$ + set

1. $t (0,1/2,1/2)$
   
2. $2 (0,0,1/2)\quad 0,1/4,z$
   
3. $c (0,0,1/2)\quad x,1/4,z$
   
4. $n (0,1/2,1/2)\quad 0,y,z$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e m'</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 d m</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 c .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 b m'm2'</td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 a mm2</td>
<td>0,0,z [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_{2a}.2mm</th>
<th>Along [1,0,0]</th>
<th>c1m11'</th>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b/2</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -a</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on mm2

Asymmetric unit: $0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/2$

Symmetry Operations

For $(0,0,0)$ + set:

1. $1\ (0,0,0)$
2. $2\ 0,0,z\ (0,0,0)$
3. $m\ x,0,z\ (m,0,0)$
4. $m\ 0,y,z\ (m,0,0)$

For $(0,1/2,1/2)' + set:

1. $t'\ (0,1/2,1/2)$
2. $2'\ 0,0,1/2\ 0,1/4,z\ (0,0,0)$
3. $c'\ (0,0,1/2)\ x,1/4,z\ (m,0,0)$
4. $n'\ (0,1/2,1/2)\ 0,y,z\ (m,0,0)$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 d m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 b mm2</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 a mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a}2mm
a* = -b/2  b* = a
Origin at 0,0,z

Along [1,0,0] c1m11'
a* = b  b* = c
Origin at x,0,0

Along [0,1,0] p1m11'
a* = -a  b* = c/2
Origin at 0,y,0
Origin on mm2

Asymmetric unit  

$$0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2$$

Symmetry Operations

For (0,0,0) + set

1. $$t \ (0,0,0)$$
   1'. $$t' \ (0,0,0')$$

2. $$2 \ (0,0,z)$$
   2'. $$2' \ (0,0,1/2)$$

3. $$m \ (x,0,z)$$
   3'. $$c' \ (0,0,1/2)$$

4. $$m \ (0,y,z)$$
   4'. $$n' \ (0,1/2,1/2)$$

For (0,1/2,1/2)' + set

1. $$t' \ (0,1/2,1/2)$$
   1'. $$t' \ (1,0,0')$$

2. $$2' \ (0,0,1/2)$$
   2'. $$2' \ (0,1/2,1/2)$$

3. $$c' \ (0,0,1/2)$$
   3'. $$a' \ (1,0,0)$$

4. $$n' \ (0,1/2,1/2)$$
   4'. $$m' \ (1/2,y,z)$$

For (1,0,0)' + set

1. $$t' \ (1,0,0)$$
   1'. $$t' \ (1,1/2,1/2)$$

2. $$2' \ (1/2,0,z)$$
   2'. $$2' \ (1,0,0')$$

3. $$a' \ (1,0,0)$$
   3'. $$n \ (1,0,1/2)$$

4. $$m' \ (1/2,y,z)$$
   4'. $$n \ (0,1/2,1/2)$$

For (1,1/2,1/2) + set

1. $$t \ (1,1/2,1/2)$$
   1'. $$t \ (1,1/2,1/2)$$

2. $$2 \ (0,0,1/2)$$
   2'. $$2 \ (1,1/2,1/2)$$

3. $$n \ (1,0,1/2)$$
   3'. $$n \ (1,1/2,1/2)$$

4. $$n \ (0,1/2,1/2)$$
   4'. $$n \ (0,1/2,1/2)$$
Generators selected  (1); t(1,0,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2)’ + (1,0,0)’ + (1,1/2,1/2)’ +</td>
<td></td>
</tr>
<tr>
<td>(0,0,0) + (0,1/2,1/2)’ + (1,0,0)’ + (1,1/2,1/2)’ +</td>
<td></td>
</tr>
<tr>
<td>16 f 1 (1) x,y,z [u,v,w] (2) x̅,y,z [u̅,v̅,w̅] (3) x̅,y,z [u̅,v̅,w̅] (4) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 e m’.. 1/2,y,z [0,v,w] 1/2,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 d m.. 0,y,z [u,0,0] 0,y,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 c .m. x,0,z [0,v,0] x,0,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 b m’m2’ 1/2,0,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 a mm2 0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] p_c2mm  Along [1,0,0] c1m11’  Along [0,1,0] p1m11’

\[
\begin{align*}
a^* &= \mathbf{a} & b^* &= \mathbf{b}/2 & a^* &= \mathbf{b} & b^* &= \mathbf{c} & a^* &= -\mathbf{a} & b^* &= \mathbf{c}/2 \\
\text{Origin at } 0,0,z & & \text{Origin at } x,0,0 & & \text{Origin at } 0,y,0
\end{align*}
\]
Origin on mm'2'  

Asymmetric unit  
0 < x < 1/2; 0 < y < 1/2; 0 < z < 1/2  

Symmetry Operations  
For (0,0,0) + set  
(1) 1  
(2) 2', 0,0,z  
(3) m', x,0,z  
(4) m 0,y,z  

For (0,1/2,1/2) + set  
(1) t (0,1/2,1/2)  
(2) 2' (0,0,1/2) 0,1/4,z  
(3) c' (0,0,1/2) x,1/4,z  
(4) n (0,1/2,1/2) 0,y,z  

For (1,0,0)' + set  
(1) t' (1,0,0)  
(2) 2 1/2,0,z  
(3) a (1,0,0) x,0,z  
(4) m' 1/2,y,z  

For (1,1/2,1/2)' + set  
(1) t' (1,1/2,1/2)  
(2) 2 (0,0,1/2) 1/2,1/4,z  
(3) n (1,0,1/2) x,1/4,z  
(4) n' (0,1/2,1/2) 1/2,y,z
Generators selected (1): t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e m'</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 d m'</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 c m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>4 b m'm'2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 a mm'2'</td>
<td>0,0,z [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'  
Along [1,0,0] c1m11'  
Along [0,1,0] p221,1m1

<table>
<thead>
<tr>
<th>a'* = a</th>
<th>b'* = b/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>a'* = b</td>
<td>b'* = c</td>
</tr>
<tr>
<td>a' = -a</td>
<td>b' = c/2</td>
</tr>
</tbody>
</table>

Origin at 1/2,0,z
Origin at x,0,0
Origin at 0,y,0
Origin on m'm2'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0)

(2) 2' 0,0,z
(2) 2 | 0,0,0)

(3) m x,0,z
(m y | 0,0,0)

(4) m' 0,y,z
(m x | 0,0,0)

For (0,1/2,1/2) + set

(1) t' (0,1/2,1/2)
(1) 0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z
(2) 2 | 0,1/2,1/2)

(3) c' (0,0,1/2) x,1/4,z
(m y | 0,1/2,1/2)

(4) n (0,1/2,1/2) 0,y,z
(m x | 0,1/2,1/2)
Continued 38.10.274

Generators selected (1); t(1,0,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<th>Coordinates</th>
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<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m'..</td>
<td>1/2,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 d m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 c ..m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 b m'm2'</td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 a m'm2'</td>
<td>0,0,z [0,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2a,2m'm'</th>
<th>Along [1,0,0]</th>
<th>c_p,1m1</th>
<th>Along [0,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = -b/2</td>
<td>b^* = a</td>
<td>a^* = b</td>
<td>b^* = c</td>
<td>a^* = -a</td>
<td>b^* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>
Origin on mm'2'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1 1 (0,0,0)
    (1 | 0,0,0)

2' 0,0,z (0,0,0)'
    (2z | 0,0,0)'

m' x,0,z (m | 0,0,0)'

m 0,y,z (m | 0,0,0)

For (0,1/2,1/2) + set

1 t' (0,1/2,1/2)
    (1 | 0,1/2,1/2)'

2 (0,0,1/2) 0,1/4,z (0,1/2,1/2)
    (2z | 0,1/2,1/2)

3 c (0,0,1/2) x,1/4,z (m | 0,1/2,1/2)

4 n' (0,1/2,1/2) 0,y,z (m | 0,1/2,1/2)'

Orthorhombic
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
</tr>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 d m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 c m'..</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>2 b mm'2'</td>
<td>1/2,0,z [u,0,0]</td>
</tr>
<tr>
<td>2 a mm'2'</td>
<td>0,0,z [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a,2mm  Along [1,0,0] c1m11'  Along [0,1,0] p2b,1m1
\(a^* = -\frac{b}{2}\)  \(b^* = a\)  \(a^* = b\)  \(b^* = c\)
Origin at 0,1/4,z  Origin at x,0,0  Origin at 0,y,0

38.11.275 - 2 - 527
Origin on m'm'2

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
2. $2 \ 0,0,z$
3. $m' \ x,0,z$
4. $m' \ 0,y,z$

For $(0,1/2,1/2)'$ + set

1. $t' \ (0,1/2,1/2)$
2. $2' \ (0,0,1/2) \ 0,1/4,z$
3. $c \ (0,0,1/2) \ x,1/4,z$
4. $n \ (0,1/2,1/2) \ 0,y,z$
Generators selected  (1); t(1,0,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(0,1/2,1/2) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e m'..</td>
<td>1/2,y,z [0,v,w]</td>
<td>1/2,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 d m'..</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 c m'..</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b m'm'2</td>
<td>1/2,0,z [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a m'm'2</td>
<td>0,0,z [0,0,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_{2a}.2m'm'</th>
<th>Along [1,0,0]</th>
<th>c_p.1m'1</th>
<th>Along [0,1,0]</th>
<th>p_{2b}.1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b/2</td>
<td>b* = a</td>
<td>a* = b b* = c</td>
<td>a* = -a</td>
<td>b* = c/2</td>
<td>a* = b b* = c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on m'2

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 (0,0,0)
(2) 2 0,0,z (m',0,0,0)
(3) m' x,0,z (m',0,0,0)
(4) m' 0,y,z (m',0,0,0)

For (0,1/2,1/2)' + set

(1) t' (0,1/2,1/2) (0,0,1/2)
(2) 2' (0,0,1/2) 0,1/4,z
(3) c (0,0,1/2) x,1/4,z
(4) n (0,1/2,1/2) 0,y,z

For (1,0,0)' + set

(1) t' (1,0,0) (1,0,0)
(2) 2' 1/2,0,z (m',1,0,0)
(3) a (1,0,0) x,0,z
(4) m 1/2,y,z

For (1,1/2,1/2) + set

(1) t (1,1/2,1/2) (1,1/2,1/2)
(2) 2 (0,0,1/2) 1/2,1/4,z (m',1,1/2,1/2)
(3) h (1,0,1/2) x,1/4,z (m',1,1/2,1/2)
(4) n' (0,1/2,1/2) 1/2,y,z (m',1,1/2,1/2)
Continued 38.13.277  A kind m'm'2

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
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<tbody>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e m..</td>
<td>(2) x',y',z [u',v',w]</td>
</tr>
<tr>
<td>8 d m'..</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 c .m'</td>
<td>(4) x',y',z [u',v',w]</td>
</tr>
<tr>
<td>4 b mm'2'</td>
<td>1/2,0,z [u,0,0]</td>
</tr>
<tr>
<td>4 a m'm'2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_c,2mm  
Along [1,0,0]  c1m11'  
Along [0,1,0]  p_c,1m1

\( a^* = a \quad b^* = b/2 \)  
\( a^* = b \quad b^* = c \)  
\( a^* = -a \quad b^* = c/2 \)  

Origin at 1/2,1/4,z  
Origin at x,0,0  
Origin at 1/2,y,0
Abm2 mm2 Orthorhombic
39.1.278 Abm2

Origin on bc2

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z
(3) m x,1/4,z
(4) b (0,1/2,0) 0,y,z

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)
(2) 2 0,0,1/2 0,1/4,z
(3) c (0,0,1/2) x,0,z
(4) c (0,0,1/2) 0,y,z

(1) 0,1/2,1/2
(2) 2 (0,0,1/2) 0,1/4,z
(3) c (0,0,1/2) x,0,z
(4) c (0,0,1/2) 0,y,z

(1) 0,1/2,1/2
(2) 2 (0,0,1/2) 0,1/4,z
(3) c (0,0,1/2) x,0,z
(4) c (0,0,1/2) 0,y,z
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,1/4,z [0,v,0]</td>
<td>x,3/4,z [0,v,0]</td>
</tr>
<tr>
<td>4 b ..2</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm  Along [1,0,0] p2a*1m1  Along [0,1,0] p1m11'  
\(a^* = a\)  \(b^* = b/2\)  \(c^* = c/2\)  
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Abm21'  mm21'  Orthorhombic  
39.2.279  Abm21'  

Origin on bc21'

Asymmetric unit  
0 < x < 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1') 1' 

(2) 2  0,0,z  
(2') 2'  0,0,z'  

(2) 2  0,0,1/2  0,1/4,z  
(2') 2'  0,0,1/2'  0,1/4,z'  

(2) 2  0,0,1/2  0,1/4,z  
(2') 2'  0,0,1/2'  0,1/4,z'  

(3) m  x,1/4,z  
(3') m'  x,1/4,z'  

(3) m  x,1/4,z  
(3') m'  x,1/4,z'  

(3) m  x,1/4,z  
(3') m'  x,1/4,z'  

(4) b  (0,1/2,0)  0,y,z  
(4) b'  (0,1/2,0)  0,y,z'  

(4) b  (0,1/2,0)  0,y,z  
(4) b'  (0,1/2,0)  0,y,z'  

For (0,1/2,1/2) + set

(1) t  (0,1/2,1/2)  
(1') t'  (0,1/2,1/2)  

(2) 2  0,0,1/2  0,1/4,z  
(2') 2'  0,0,1/2'  0,1/4,z'  

(2) 2  0,0,1/2  0,1/4,z  
(2') 2'  0,0,1/2'  0,1/4,z'  

(2) 2  0,0,1/2  0,1/4,z  
(2') 2'  0,0,1/2'  0,1/4,z'  

(3) c  (0,0,1/2)  x,0,z  
(3') c'  (0,0,1/2)  x,0,z'  

(3) c  (0,0,1/2)  x,0,z  
(3') c'  (0,0,1/2)  x,0,z'  

(3) c  (0,0,1/2)  x,0,z  
(3') c'  (0,0,1/2)  x,0,z'  

(4) c  (0,0,1/2)  0,y,z  
(4') c'  (0,0,1/2)  0,y,z'  

(4) c  (0,0,1/2)  0,y,z  
(4') c'  (0,0,1/2)  0,y,z'  

For (0,0,0)' + set

(1) t' (0,1/2,1/2)'  
(1') t (0,1/2,1/2) 

(2) 2'  0,0,z'  
(2) 2  0,0,z  

(2) 2'  0,0,z'  
(2) 2  0,0,z  

(2) 2'  0,0,z'  
(2) 2  0,0,z  

(3) m'  x,1/4,z'  
(3) m  x,1/4,z  

(3) m'  x,1/4,z'  
(3) m  x,1/4,z  

(3) m'  x,1/4,z'  
(3) m  x,1/4,z  

(4) b'  (0,1/2,0)  0,y,z'  
(4) b  (0,1/2,0)  0,y,z  

(4) b'  (0,1/2,0)  0,y,z'  
(4) b  (0,1/2,0)  0,y,z  

(4) b'  (0,1/2,0)  0,y,z'  
(4) b  (0,1/2,0)  0,y,z  

For (0,1/2,1/2)' + set

(1) t' (0,1/2,1/2) 
(1') t (0,1/2,1/2) 

(2) 2'  0,0,1/2'  0,1/4,z'  
(2) 2  0,0,1/2  0,1/4,z  

(2) 2'  0,0,1/2'  0,1/4,z'  
(2) 2  0,0,1/2  0,1/4,z  

(2) 2'  0,0,1/2'  0,1/4,z'  
(2) 2  0,0,1/2  0,1/4,z  

(3) c'  (0,0,1/2)  x,0,z  
(3') c  (0,0,1/2)  x,0,z'  

(3) c'  (0,0,1/2)  x,0,z  
(3') c  (0,0,1/2)  x,0,z'  

(3) c'  (0,0,1/2)  x,0,z  
(3') c  (0,0,1/2)  x,0,z'  

(4) c'  (0,0,1/2)  0,y,z  
(4) c  (0,0,1/2)  0,y,z'  

(4) c'  (0,0,1/2)  0,y,z  
(4) c  (0,0,1/2)  0,y,z'  

(4) c'  (0,0,1/2)  0,y,z  
(4) c  (0,0,1/2)  0,y,z'  

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**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (0,0,0)’ + (0,1/2,1/2)’ +</td>
<td>(0,0,0) + (0,1/2,1/2) + (0,0,0)’ + (0,1/2,1/2)’ +</td>
</tr>
<tr>
<td>8 d  11’  (1) x,y,z [0,0,0]  (2) x,y,z [0,0,0]  (3) x,y+1/2,z [0,0,0]  (4) x,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 c  .m.1’  x,1/4,z [0,0,0]</td>
<td>x,3/4,z [0,0,0]</td>
</tr>
<tr>
<td>4 b  .21’  1/2,0,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 a  .21’  0,0,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]  p2mm1’</th>
<th>Along [1,0,0]  p1m11’</th>
<th>Along [0,1,0]  p1m11’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a  b* = b/2</td>
<td>a* = b/2  b* = c/2</td>
<td>a* = -a  b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin on b'c2'

Asymmetric unit

\[
0 < x < 1/2; \quad 0 < y < 1/4; \quad 0 < z < 1
\]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2', 0,0,z \\
(3) & \quad m, x,1/4,z \\
(4) & \quad b', (0,1/2,0), 0,y,z
\end{align*}
\]

For (0,1/2,1/2) + set

\[
\begin{align*}
(1) & \quad t, (0,1/2,1/2) \\
(2) & \quad 2', (0,0,1/2), 0,1/4,z \\
(3) & \quad c, (0,0,1/2), x,0,z \\
(4) & \quad c', (0,0,1/2), 0,y,z
\end{align*}
\]
Continued

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>c m.</td>
<td>x,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>4</td>
<td>b m.</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4</td>
<td>a m.</td>
<td>0,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  
**p2'mm'**

- \( \mathbf{a}^* = -b/2 \)
- \( \mathbf{b}^* = a \)
- Origin at 0,0,z

Along [1,0,0]  
**p1m1**

- \( \mathbf{a}^* = b/2 \)
- \( \mathbf{b}^* = c/2 \)
- Origin at 0,0,z

Along [0,1,0]  
**p1m11'**

- \( \mathbf{a}^* = -a \)
- \( \mathbf{b}^* = c/2 \)
- Origin at 0,y,0
Abm'2' mm'2' Orthorhombic

39.4.281 Abm'2'

Origin on bc'2'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) +\) set

1. \(1\)\( (1|0,0,0) \)
2. \(2'\) \(0,0,z\) \( (2_z|0,0,0)' \)
3. \(m'\) \(x,1/4,z\) \( (m_y|0,1/2,0)' \)
4. \(b\) \((0,1/2,0)\) \(0,y,z\) \( (m_z|0,1/2,0) \)

For \((0,1/2,1/2) +\) set

1. \(t\) \((0,1/2,1/2)\) \( (1|0,1/2,1/2) \)
2. \(2'\) \((0,0,1/2)\) \(0,1/4,z\) \((2_z|0,1/2,1/2)' \)
3. \(c'\) \((0,0,1/2)\) \(x,0,z\) \( (m_y|0,0,1/2)' \)
4. \(c\) \((0,0,1/2)\) \(0,y,z\) \( (m_z|0,0,1/2) \)
Generators selected

(1); t(1,0,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td></td>
</tr>
<tr>
<td>(0,1/2,1/2) +</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>d 1</th>
<th>(1) x,y,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y+1/2,z [u,v,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>c .m'</th>
<th>x,1/4,z [u,0,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>x,1/4,z [u,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,1/2,z [u,v,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>b ..2'</th>
<th>0,0,z [u,v,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0,1/2,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2'2mm'</th>
<th>Along [1,0,0]</th>
<th>p_2a.1m1</th>
<th>Along [0,1,0]</th>
<th>p1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b/2</td>
<td>a* = b/2</td>
<td>b* = c/2</td>
<td>a* = -a</td>
<td>b* = c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z |

Origin at x,0,0 |

Origin at 0,y,0 |
Ab’m’2 Orthorhombic

39.5.282

Origin on b’c’2

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z
   (2z 0,0,0)
(3) m’ x,1/4,z
   (m,0,1/2,0)'
(4) b’ (0,1/2,0) 0,y,z
   (m,0,1/2,0)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)
   (1 0,1/2,1/2)
(2) 2 (0,0,1/2) 0,1/4,z
   (2z 0,1/2,1/2)
(3) c’ (0,0,1/2) x,0,z
   (m,0,0,1/2)'
(4) c’ (0,0,1/2) 0,y,z
   (m,0,0,1/2)’
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w] (2) ( \bar{x}, \bar{y}, z [\bar{u}, \bar{v}, \bar{w}] ) (3) ( x, y+1/2, z [u,v,w] ) (4) ( \bar{x}, y+1/2, z [\bar{u}, \bar{v}, \bar{w}] )</td>
</tr>
<tr>
<td>4 c .m'</td>
<td>x,1/4,z [u,0,w] ( \bar{x}, 3/4,z [\bar{u},0,w] )</td>
</tr>
<tr>
<td>4 b ..2</td>
<td>1/2,0,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w] 0,1/2,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'
\( a^* = a \ b^* = b/2 \)
Origin at 0,0,z

Along [1,0,0] p1m'1
\( a^* = b/2 \ b^* = c/2 \)
Origin at x,0,0

Along [0,1,0] p1m'1
\( a^* = -a \ b^* = c/2 \)
Origin at 0,y,0
Origin on bc2

Asymmetric unit
\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0) + \) set

(1) \(I\)
(1) \((0,0,0)\)
(1) \((1,0,0)\)
(1) \((1,0,0)\)'

(2) \(2\)
(2) \(0,0,z\)
(2) \(0,0,1/2\)
(2) \(0,0,1/2\)' \\
\((2z|0,0,0)\)
\((2z|0,0,1/2)\)
\((2z|1,0,0)\)'
\((2z|1,0,0)\)''

(3) \(m\)
(3) \(x,1/4,z\)
(3) \(c,0,0,1/2\)
(3) \(a',1,0,0\)

\((m|0,1/2,0)\)
\((m|0,0,1/2)\)
\((m|1,1/2,0)\)'
\((m|1,1/2,0)\)''

(4) \(b\)
(4) \((0,1/2,0)\)
(4) \((0,0,1/2)\)
(4) \((0,0,1/2)\)'

\((m|0,1/2,0)\)
\((m|0,0,1/2)\)
\((m|1,1/2,0)\)'
\((m|1,1/2,0)\)''

For \((0,1/2,1/2) + \) set

(1) \(t\)
(1) \((0,1/2,1/2)\)
(1) \((0,1/2,1/2)\)'

(2) \(2\) \(0,0,1/2\) \(0,1/4,z\)
(2) \(0,0,1/2\) \(0,1/4,z\)
(2) \(0,0,1/2\) \(0,1/4,z\)

\((2z|0,0,1/2)\)
\((2z|0,1/2,1/2)\)
\((2z|1,0,0)\)'

(3) \(c\)
(3) \((0,0,1/2)\) \(x,0,z\)
(3) \((0,0,1/2)\) \(x,0,z\)

\((m|0,0,1/2)\)
\((m|0,0,1/2)\)
\((m|0,0,1/2)\)

(4) \(c\)
(4) \((0,0,1/2)\) \(0,y,z\)
(4) \((0,0,1/2)\) \(0,y,z\)

\((m|0,0,1/2)\)
\((m|0,0,1/2)\)
\((m|0,0,1/2)\)

For \((1,0,0)'+ \) set

(1) \(t'\)
(1) \((1,0,0)\)
(1) \((1,0,0)\)'

(2) \(2'\)
(2) \((1/2,0)\) \(0,z\)
(2) \((1/2,0)\) \(0,z\)

\((2z|1,0,0)\)'
\((2z|1,0,0)\)''
\((2z|1,0,0)\)''

(3) \(a'\)
(3) \((1,0,0)\) \(x,1/4,z\)
(3) \((1,0,0)\) \(x,1/4,z\)

\((m|1,1/2,0)\)'
\((m|1,1/2,0)\)''
\((m|1,1/2,0)\)''

(4) \(b'\)
(4) \((0,1/2,0)\) \(1/2,y,z\)
(4) \((0,1/2,0)\) \(1/2,y,z\)

\((m|1,1/2,0)\)'
\((m|1,1/2,0)\)''
\((m|1,1/2,0)\)''

For \((1,1/2,1/2)'+ \) set

(1) \(t'\)
(1) \((1/2,1/2)\)
(1) \((1/2,1/2)\)'

(2) \(2'\)
(2) \((1/2,1/2)\) \(0,1/4,z\)
(2) \((1/2,1/2)\) \(0,1/4,z\)

\((2z|1,1/2,1/2)\)'
\((2z|1,1/2,1/2)\)''
\((2z|1,1/2,1/2)\)''

(3) \(n'\)
(3) \((1,1/2,1/2)\) \(x,0,z\)
(3) \((1,1/2,1/2)\) \(x,0,z\)

\((m|1,0,1/2)\)'
\((m|1,0,1/2)\)''
\((m|1,0,1/2)\)''

(4) \(c'\)
(4) \((0,0,1/2)\) \(1/2,y,z\)
(4) \((0,0,1/2)\) \(1/2,y,z\)

\((m|1,0,1/2)\)'
\((m|1,0,1/2)\)''
\((m|1,0,1/2)\)''

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Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 c .m.</td>
<td>x,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>8 b ..2'</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 a ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p2a 2mm</td>
<td>0,0,z</td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p1m11'</td>
<td>x,0,0</td>
</tr>
<tr>
<td>[0,1,0]</td>
<td>p1m11'</td>
<td>0,y,0</td>
</tr>
</tbody>
</table>
Origin on bc'2

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) 0,0,0

(3) m x,1/4,z
(m) 0,1/2,0

(4) b (0,1/2,0) 0,y,z
(m) 0,1/2,0

For (0,1/2,1/2)' + set

(1) t' (0,0,1/2)
(1) 0,1/2,1/2)'

(2) 2' (0,0,1/2) 0,1/4,z
(2) 0,1/2,1/2)' (m) 0,1/2,0

(3) c' (0,0,1/2) x,0,z
(m) 0,0,1/2)' (m) 0,0,1/2)

(4) c' (0,0,1/2) 0,y,z
(m) 0,0,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (0,1/2,1/2)' +

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,1/2,1/2)' +</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,1/4,z [0,v,0]</td>
<td>x,3/4,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 b ..2</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a*}2mm  
Origin at 0,0,z  
\(a^* = -b/2, b^* = a\)

Along [1,0,0] p_{2a*}1m1  
Origin at x,1/4,0  
\(a^* = b/2, b^* = c/2\)

Along [0,1,0] p_{1m11'}  
Origin at 0,y,0  
\(a^* = -a, b^* = c/2\)
Origin on bc'2

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

1. $t (0,0,0)$
2. $0,0,z$
3. $m x,1/4,z$
4. $b (0,1/2,0) 0,y,z$

For (0,1/2,1/2)' + set

1. $t' (0,1/2,1/2)$
2. $0,0,1/2$ 0,1/4,z
3. $c' (0,0,1/2) x,0,z$
4. $c' (0,0,1/2) 0,y,z$

For (1,0,0)' + set

1. $t' (1,0,0)$
2. $1/2,0,z$
3. $a' (1,0,0) x,1/4,z$
4. $b' (0,1/2,0) 1/2,y,z$

For (1,1/2,1/2) + set

1. $t (1,1/2,1/2)$
2. $0,0,1/2$ 1/2,1/4,z
3. $n (1,0,1/2) x,0,z$
4. $c (0,0,1/2) 1/2,y,z$
Generators selected  \( (1); \ t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ t(0,1/2,1/2); \ (2); \ (3). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1,0,0)' + (0,1,0)' + (1,1/2,1/2) +</td>
<td>(0,1/2,1/2)' + (1,1/2,1/2) +</td>
</tr>
<tr>
<td>16 d 1 (1) x,y,z [u,v,w] (2) x,y+1/2,z [u,v,w] (3) x,y+1/2,z [u,v,w] (4) x,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 c .m. x,1/4,z [0,v,0] 1/2,1/2,1/2 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 b .2' 1/2,0,z [u,v,0] 1/2,1/2,2 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 a .2 0,0,z [0,0,w] 0,1/2,2 [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]** \( p_{c2}mm \) \( a^* = a \ b^* = b/2 \) Origin at 1/2,1/4,z
- **Along [1,0,0]** \( p1m11' \) \( a^* = b/2 \ b^* = c/2 \) Origin at x,0,0
- **Along [0,1,0]** \( p1m11' \) \( a^* = -a \ b^* = c/2 \) Origin at 0,y,0
Orthorhombic

$A_{2a} b'm'2$

$mm21'$

39.9.286

$A_{2a} b'm'2$

Origin on $b'c'2$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

1. $t (1,0,0)$
   2. $t' (1,1/2,1/2)$
   3. $t' (1,1/2,1/2)$

For $(0,1/2,1/2) +$ set

1. $t (0,0,1/2)$
   2. $t (0,0,1/2)$
   3. $t (0,0,1/2)$

For $(1,0,0)' +$ set

1. $t (1,0,0)$
   2. $t (1,0,0)$
   3. $t (1,0,0)$

For $(1,1/2,1/2)' +$ set

1. $t (0,0,1/2)$
   2. $t (0,0,1/2)$
   3. $t (0,0,1/2)$

For $(0,0,0)' +$ set

1. $t (1,0,0)$
   2. $t (1,0,0)$
   3. $t (1,0,0)$

For $(0,1/2,1/2)' +$ set

1. $t (0,0,1/2)$
   2. $t (0,0,1/2)$
   3. $t (0,0,1/2)$

For $(1,0,0)' +$ set

1. $t (1,0,0)$
   2. $t (1,0,0)$
   3. $t (1,0,0)$

For $(1,1/2,1/2)' +$ set

1. $t (0,0,1/2)$
   2. $t (0,0,1/2)$
   3. $t (0,0,1/2)$
Continued

Generators selected (1); t(1,0,0)'; t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

| Multiplicity, Wyckoff letter, Site Symmetry. |
|-----------------|------------------|
| 16 d 1          | (1) x,y,z [u,v,w] (2) \( \bar{x}, y, z [\bar{u}, \bar{v}, \bar{w}] \) (3) \( x, y^+1/2, z [u, \bar{v}, \bar{w}] \) (4) \( x, y+1/2, z [\bar{u}, v, \bar{w}] \) |
| 8 c .m'         | x,1/4,z [u,0,w]  \( \bar{x}, 3/4, z [\bar{u}, 0, w] \) |
| 8 b ..2'        | 1/2,0,z [u,v,0]  1/2,1/2,z [\bar{u}, \bar{v}, 0] |
| 8 a ..2         | 0,0,z [0,0,w]     0,1/2,z [0,0,w] |

Symmetry of Special Projections

Along [0,0,1] p2m'm' \( a^* = a \ b^* = b/2 \) Origin at 0,0,z
Along [1,0,0] p1m11' \( a^* = b/2 \ b^* = c/2 \) Origin at x,0,0
Along [0,1,0] p2\(2_{\text{v}}.1m1 \) \( a^* = -a \ b^* = c/2 \) Origin at 1/2,y,0
**Origin**  
on b’c’2’

**Asymmetric unit**  
0 ≤ x ≤ 1/2;  
0 ≤ y ≤ 1/4;  
0 ≤ z ≤ 1

**Symmetry Operations**

For (0,0,0) + set

1. \(1\) \(0,0,0\)  

2. \(2'\) \(0,0,z\)  
\(2_z\) \(0,0,0'\)

3. \(m\) \(x,1/4,z\)  
\(m_y\) \(0,1/2,0\)

4. \(b'\) \(0,1/2,0\)  
\(m_x\) \(0,1/2,0'\)

For (0,1/2,1/2)’ + set

1. \(t'\) \(0,1/2,1/2\)
\(t'\) \(0,1/2,1/2'\)

2. \(2\) \(0,0,1/2\)  
\(2_z\) \(0,1/2,1/2\)

3. \(c'\) \(0,0,1/2\)  
\(m_y\) \(0,0,1/2'\)

4. \(c\) \(0,0,1/2\)  
\(m_x\) \(0,0,1/2\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2)' +</td>
<td></td>
</tr>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c m.</td>
<td>x,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>4 b 2'</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 a 2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a2mm
a* = -b/2  b* = a
Origin at 0,1/4,z

Along [1,0,0] p1m1
a* = b/2  b* = c/2
Origin at x,0,0

Along [0,1,0] p1m11'
a* = -a  b* = c/2
Origin at 0,y,0
Origin on bc2'

Asymmetric unit  
\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
2. \(2' 0,0,z\)
3. \(m' x,\frac{1}{4},z\)
4. \(b (0,1/2,0) 0,y,z\)

\(\text{For } (0,1/2,1/2)' + \text{ set}\)

1. \(t' (0,1/2,1/2)\)
2. \(2 (0,0,1/2) 0,1/4,z\)
3. \(c (0,0,1/2) x,0,z\)
4. \(c' (0,0,1/2) 0,y,z\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity,        Coordinates
Wyckoff letter,      (0,0,0) + (0,1/2,1/2)'
Site Symmetry.       +

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x̅,y̅,z [u,v̅,w]</td>
</tr>
<tr>
<td>4 c m'</td>
<td>x,1/4,z [u,0,w]</td>
<td>x̅,3/4,z [u,0,w̅]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,1/2,z [u,v̅,0]</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>0,0,z [u,v,0]</td>
<td>0,1/2,z [u,v̅,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a-2m'm'}  
\( \mathbf{a}^* = -b/2 \)  \( \mathbf{b}^* = a \)
Origin at 0,1/4,z

Along [1,0,0] p_{2a-1m1}  
\( \mathbf{a}^* = b/2 \)  \( \mathbf{b}^* = c/2 \)
Origin at x,0,0

Along [0,1,0] p_{2v-1m1}  
\( \mathbf{a}^* = -a \)  \( \mathbf{b}^* = c/2 \)
Origin at 0,y,0
Origin on b'c2

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

1) 1
   (1 0,0,0)
2) 2 0,0,z
   (2 0,0,0)
3) m' x,1/4,z
   (m 0,1/2,0)
4) b' (0,1/2,0) 0,y,z
   (m 0,1/2,0)

For (0,1/2,1/2)' + set

1) t' (0,1/2,1/2)
   (1 0,1/2,1/2)
   (1 0,1/2,1/2)
2) 2' (0,0,1/2) 0,1/4,z
   (2 0,1/2,1/2)
   (2 0,1/2,1/2)
3) c (0,0,1/2) x,0,z
   (m 0,0,1/2)
4) c (0,0,1/2) 0,y,z
   (m 0,0,1/2)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .m'</td>
<td>x,1/4,z [u,0,w]</td>
</tr>
<tr>
<td>4 b .2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2v}2mm

a* = -b/2  b* = a
Origin at 0,0,z

Along [1,0,0] p_{1m'1}

a* = b/2  b* = c/2
Origin at x,0,0

Along [0,1,0] p_{2v}1m'1

a* = -a  b* = c/2
Origin at 0,y,0
Origin on b’c2

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1 0,0,0)
(2) 2 0,0,z
    (2z 0,0,0)
(3) m’ x,1/4,z
    (mz 0,1/2,0)'
(4) b’ (0,1/2,0) 0,y,z
    (mz 0,1/2,0)'

For (0,1/2,1/2)’ + set

(1) t’ (0,1/2,1/2)
    (1 0,1/2,1/2)’
(2) 2’ (0,0,1/2) 0,1/4,z
    (2z 0,1/2,1/2)’
(3) c (0,0,1/2) x,0,z
    (mz 0,0,1/2)
(4) c (0,0,1/2) 0,y,z
    (mz 0,0,1/2)

For (1,0,0)’ + set

(1) t’ (1,0,0)
    (1 1,0,0)’
(2) 2’ 1/2,0,z
    (2z 1,0,0)’
(3) a (1,0,0) x,1/4,z
    (mz 1,1/2,0)
(4) b (0,1/2,0) 1/2,y,z
    (mz 1,1/2,0)

For (1,1/2,1/2) + set

(1) t (1,1/2,1/2)
    (1 1,1/2,1/2)
(2) 2 (0,0,1/2) 1/2,1/4,z
    (2z 1,1/2,1/2)
(3) n’ (1,0,1/2) x,0,z
    (mz 1,0,1/2)’
(4) c’ (0,0,1/2) 1/2,y,z
    (mz 1,0,1/2)’
Generators selected  \( (1); t(1,0,0)'; t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 d 1</td>
<td>((0,0,0) + (0,1/2,1/2)' + (1,0,0)' + (1,1/2,1/2) + )</td>
</tr>
<tr>
<td>8 c .m'</td>
<td>((0,1,0,0) + )</td>
</tr>
<tr>
<td>8 b ..2'</td>
<td>((1,0,0,0) + )</td>
</tr>
<tr>
<td>8 a ..2</td>
<td>((0,0,0,0) + )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\)  \(p_{\text{c}}2\text{mm}\)  \(a^* = a  b^* = b/2\)  Origin at 0,0,z

Along \([1,0,0]\)  \(p_{\text{1m}11}'\)  \(a^* = b/2  b^* = c/2\)  Origin at x,0,0

Along \([0,1,0]\)  \(p_{\text{c}}1\text{m1}\)  \(a^* = -a  b^* = c/2\)  Origin at 1/2,y,0
Origin on 1a2

Asymmetric unit

\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1\]

Symmetry Operations

For \((0,0,0) + \) set

(1) \(1\)

(2) \(2, 0,0,z\)

(3) \(a (1/2,0,0) x,0,z\)

(4) \(m 1/4,y,z\)

\((m_x) 1/2,0,0)\)

For \((0,1/2,1/2) + \) set

(1) \(t (0,1/2,1/2)\)

(2) \(2 (0,0,1/2) 0,1/4,z\)

(3) \(n (1/2,0,1/2) x,1/4,z\)

(4) \(n (0,1/2,1/2) 1/4,y,z\)

\((m_x) 1/2,1/2,1/2)\)
Generators selected (1); t(1,0,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x+1/2,y,z [u,v,w] (4) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>1/4,y,z [u,0,0] 3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>0,0,z [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2mg</th>
<th>Along [1,0,0]</th>
<th>c1m11'</th>
<th>Along [0,1,0]</th>
<th>p2a1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b/2)</td>
<td>(a^* = b) (b^* = c)</td>
<td>(a^* = -a/2) (b^* = c/2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 1/4,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The document contains information about the crystal structure of a material with the space group Ama21'. The diagram and text provide details about the origin, asymmetric unit, and symmetry operations for this structure.

**Origin**: on 1a21'

**Asymmetric unit**: $0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

**Symmetry Operations**

For $(0,0,0)$ + set:

1. $1$
2. $2 \ 0,0,z$
3. $a \ (1/2,0,0) \ x,0,z$
4. $m \ 1/4,y,z$

For $(0,1/2,1/2)$ + set:

1. $t \ (0,1/2,1/2)$
2. $2 \ (0,0,1/2) \ 0,1/4,z$
3. $n \ (1/2,0,1/2) \ x,1/4,z$
4. $n' \ (0,1/2,1/2) \ 1/4,y,z$

For $(0,0,0)'$ + set:

1. $1'$
2. $2' \ 0,0,z$
3. $a' \ (1/2,0,0) \ x,0,z$
4. $m' \ 1/4,y,z$

For $(0,1/2,1/2)'$ + set:

1. $t' \ (0,1/2,1/2)$
2. $2' \ (0,0,1/2) \ 0,1/4,z$
3. $n' \ (1/2,0,1/2) \ x,1/4,z$
4. $n' \ (0,1/2,1/2) \ 1/4,y,z$
Generators selected  (1); t(1,0,0); t(0,0,0); t(0,0,1); t(0,1/2,1/2); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c</td>
<td>11' (1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>m..1' 1/4,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>..21' 0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg1'  Along [1,0,0] c1m11'  Along [0,1,0] p1m11'

\[ a^* = a \quad b^* = b/2 \]
\[ a^* = b \quad b^* = c \]
\[ a^* = -a/2 \quad b^* = c/2 \]

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Am'a2' m'm2' Orthorhombic

40.3.293 Am'a2'

**Origin** on 1a2'

**Asymmetric unit**

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1 \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1\)
   
   \((1|0,0,0)\)

2. \(2'\)
   
   \((2_z|0,0,0)\)

3. \(a\)
   
   \((1/2,0,0)\)

4. \(m'\)
   
   \((1/4,y,z)\)

For \((0,1/2,1/2)\) + set

1. \(t\)
   
   \((0,1/2,1/2)\)

2. \(2'\)
   
   \((0,0,1/2)\)

3. \(n\)
   
   \((1/2,0,1/2)\)

4. \(n'\)
   
   \((0,1/2,1/2)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
<td></td>
</tr>
<tr>
<td>4 b m'..</td>
<td>1/4,y,z [0,v,w]</td>
<td>(0,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>0,0,z [u,v,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2'm'g  
\( a^* = a \quad b^* = b/2 \)
Origin at 0,0,z

Along [1,0,0]  c1m1  
\( a^* = b \quad b^* = c \)
Origin at x,0,0

Along [0,1,0]  p_{2a}.1m1  
\( a^* = -a/2 \quad b^* = c/2 \)
Origin at 0,y,0
**Origin**  on 1a'2'

**Asymmetric unit**  
0 ≤ x < 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z < 1

**Symmetry Operations**

For (0,0,0) + set

1. \( l (1,0,0,0) \)  
2. \( 2' (0,0,z) \)
3. \( a' (1/2,0,0) x,0,z \)
4. \( m 1/4,y,z \)

For (0,1/2,1/2) + set

1. \( t (0,1/2,1/2) \)  
2. \( 2' (0,0,1/2) 0,1/4,z \)
3. \( n' (1/2,0,1/2) x,1/4,z \)
4. \( n (0,1/2,1/2) 1/4,y,z \)

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Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

(0,0,0) + (0,1/2,1/2) +

<table>
<thead>
<tr>
<th>8</th>
<th>c</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) x+1/2,y,z [u,v,w]</th>
<th>(4) x+1/2,y,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>b</td>
<td>m., 1/4,y,z [u,0,0]</td>
<td>3/4, y,z [u,0,0]</td>
<td>1/2,0,z [u,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>..2', 0,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2'mg'  Along [1,0,0]  c1m11'  Along [0,1,0]  p1m1

a* = a  b* = b/2  a* = b  b* = c  a* = -a/2  b* = c/2

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on \(1\alpha'2\)

Asymmetric unit \(0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \ \ 1 & (2) & \ (0,0,z) & (3) & \ (1/2,0,0) & (4) & \ m' \\
(1) & \ (0,0,0) & (2) & \ (0,0,0) & (3) & \ (1/2,0,0)' & (4) & \ m' \\
\end{align*}
\]

For \((0,1/2,1/2) + \) set

\[
\begin{align*}
(1) & \ t (0,1/2,1/2) & (2) & \ (0,1/2,1/2) & (3) & \ (1/2,0,1/2) & (4) & \ n' \\
(1) & \ (0,1/2,1/2) & (2) & \ (0,1/2,1/2) & (3) & \ (1/2,1/2,1/2)' & (4) & \ n' \\
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

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<th>Site Symmetry</th>
</tr>
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<tr>
<td>8 c 1</td>
<td>1 x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>4 b m'..</td>
<td>1/4,y,z [0,v,w]</td>
<td>(0,1/2,1/2) +</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Coordinates

(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) x+1/2,y,z [u,v,w]  (4) x+1/2,y,z [u,v,w]

Symmetry of Special Projections

Along [0,0,1]  p2m'g'  a* = a  b* = b/2  Origin at 0,0,z
Along [1,0,0]  c1m'1  a* = b  b* = c  Origin at x,0,0
Along [0,1,0]  p1m'1  a* = -a/2  b* = c/2  Origin at 0,y,0
Origin on 1a2

Asymmetric unit $0 \leq x \leq 1/4$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1
(1) $0,0,0$
(1) $0,0,0$

(2) 2 0,0,z
(2) $0,0,0$
(2) $0,0,0$

(3) a $(1/2,0,0)$ x,0,z
(3) $(m_y|1/2,0,0)$
(3) $(m_y|1/2,0,0)$

(4) m 1/4,y,z
(4) $(m_y|1/2,0,0)$
(4) $(m_y|1/2,0,0)$

For $(0,1/2,1/2)^{+}$ set

(1) $t^\prime$ $(0,1/2,1/2)$
(1) $(0,1/2,1/2)$
(1) $(0,1/2,1/2)$

(2) $2^\prime$ $(0,0,1/2)$ 0,1/4,z
(2) $(0,1/2,1/2)^\prime$
(2) $(0,1/2,1/2)^\prime$

(3) $n^\prime$ $(1/2,0,1/2)$ x,1/4,z
(3) $(m_y|1/2,1/2)^\prime$
(3) $(m_y|1/2,1/2)^\prime$

(4) $n^\prime$ $(0,1/2,1/2)$ 1/4,y,z
(4) $(m_y|1/2,1/2)^\prime$
(4) $(m_y|1/2,1/2)^\prime$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b m..</td>
<td>1/4,y,z [u,0,0]</td>
<td>3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{2\alpha} \cdot 2mg \) Along [1,0,0] \( c1m11' \) Along [0,1,0] \( p_{c} \cdot 1m1 \)
\( a^* = a \quad b^* = b/2 \) \( a^* = b \quad b^* = c \) \( a^* = -a/2 \quad b^* = c/2 \)
Origin at 0,0,z Origin at x,0,0 Origin at 1/4,y,0
Origin on 1a2'

Asymmetric unit:

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations:

For (0,0,0) + set:

1. [0,0,0]
2. 2', 0,0,z
3. a (1/2,0,0) x,0,z
4. m' 1/4,y,z

For (0,1/2,1/2)' + set:

1. t' (0,1/2,1/2)
2. 2 (0,0,1/2) 0,1/4,z
3. n' (1/2,0,1/2) x,1/4,z
4. n (0,1/2,1/2) 1/4,y,z
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3). \)

### Positions

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<tr>
<td>( 8 ) c 1</td>
<td>( (1) x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>( 4 ) b m'</td>
<td>( 1/4,y,z [0,v,w] )</td>
</tr>
<tr>
<td>( 4 ) a ..2'</td>
<td>( 0,0,z [u,v,0] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along \([0,0,1]\) \( p_{2vb}'2m'g' \)
- Along \([1,0,0]\) \( c_{p,1}m1 \)
- Along \([0,1,0]\) \( p_{c,1}m1 \)

<table>
<thead>
<tr>
<th>Origin at ( 0,1/4,z )</th>
<th>( a^* = a ) ( b^* = b/2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at ( x,0,0 )</td>
<td>( a^* = b ) ( b^* = c )</td>
</tr>
<tr>
<td>Origin at ( 1/4,y,0 )</td>
<td>( a^* = -a/2 ) ( b^* = c/2 )</td>
</tr>
</tbody>
</table>
Origin on 1a'2'

Asymmetric unit

\[ 0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1 \]

Symmetry Operations

For \((0,0,0) + \text{ set}\)

\[
(1) \quad t \quad (0,0,0)
\]

\[
(2) \quad 2' \quad 0,0,z

(2)_{z} \quad 0,0,0')
\]

\[
(3) \quad a' (1/2,0,0) \quad x,0,z

(m_{y})_{1/2,0,0')}
\]

\[
(4) \quad m \quad 1/4,y,z

(m_{x})_{1/2,0,0'}
\]

For \((0,1/2,1/2') + \text{ set}\)

\[
(1) \quad t' (0,1/2,1/2)

(1)_{z} (0,1/2,1/2')
\]

\[
(2) \quad 2 (0,0,1/2) \quad 0,1/4,z

(2)_{z} (0,1/2,1/2')
\]

\[
(3) \quad n (1/2,0,1/2) \quad x,1/4,z

(m_{y})_{1/2,1/2,1/2}
\]

\[
(4) \quad n' (0,1/2,1/2) \quad 1/4,y,z

(m_{x})_{1/2,1/2,1/2'}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2)'; (2); (3).

Positions

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<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>4 b m..</td>
<td>1/4,y,z [u,0,0]</td>
<td>3/4,y,z [u,0,0]</td>
<td>(0,1/2,1/2)'+</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>0,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2,v.2mg  
Along [1,0,0]  c1m11'  
Along [0,1,0]  p2,v.1m1  

\( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b}/2 \)  
\( \mathbf{a}^* = \mathbf{b} \)  \( \mathbf{b}^* = \mathbf{c} \)

Origin at 0,1/2,z  
Origin at x,0,0  
Origin at 0,y,0
Origin on 1a'2

Asymmetric unit $0 \leq x \leq 1/4$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) $1$
(1) $t'$ (0,1/2,1/2)
(1) $0,0,0$
(1) $0,0,0$
(1) $0,0,0$
(1) $t'$ (0,1/2,1/2)

(2) $0,0,z$
(2) $0,0,0$ (m)$\frac{1}{2},0,0$
(2) $0,0,0$ (m)$\frac{1}{2},0,0$
(2) $0,0,0$ (m)$\frac{1}{2},0,0$
(2) $0,0,0$ (m)$\frac{1}{2},0,0$

(3) $a'$ (1/2,0,0) x,0,z
(3) $n$ (1/2,0,1/2) x,1/4,z
(3) $n$ (1/2,0,1/2) x,1/4,z
(3) $n$ (1/2,0,1/2) x,1/4,z

(4) $m'$ 1/4,y,z
(4) $m'$ 1/4,y,z
(4) $m'$ 1/4,y,z
(4) $m'$ 1/4,y,z
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>8</td>
<td>c 1</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>4</td>
<td>b m'..</td>
<td>1/4, y, z [0, v, w]</td>
</tr>
<tr>
<td>4</td>
<td>a ..2</td>
<td>0, 0, z [0, 0, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  $p_{2v}.2m'g'$  \[ a^* = a \quad b^* = b/2 \]
Origin at 0,0,z

Along [1,0,0]  $c_{1}m'1$  \[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [0,1,0]  $p_{2v}.1m'1$  \[ a^* = -a/2 \quad b^* = c/2 \]
Origin at 0,y,0
Origin on 1n2

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
   1 | $0,0,0$
2. $2$
   z | $0,0,0$
3. a | $(1/2,0,0)$ $x,1/4,z$
   (m) | $1/2,1/2,0$
4. b | $(0,1/2,0)$ $1/4,y,z$
   (m) | $1/2,1/2,0$

For $(0,1/2,1/2)$ + set

1. t | $(0,1/2,1/2)$
   1 | $0,1/2,1/2$
2. $2$
   z | $(0,0,1/2)$ $0,1/4,z$
   (m$,$) | $1/2,1/2,1/2$
3. n | $(1/2,0,1/2)$ $x,0,z$
   (m$,$) | $1/2,0,1/2$
4. c | $(0,0,1/2)$ $1/4,y,z$
   (m$,$) | $1/2,0,1/2$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

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<th>Site Symmetry</th>
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<tr>
<td>(0,0,0) +</td>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
<td>(2) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg
\[ \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b}/2 \]
Origin at 0,0,z

Along [1,0,0] p_{2a.m'}1
\[ \mathbf{a}^* = \mathbf{b}/2, \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x,0,0

Along [0,1,0] p_{2a.1m'}1
\[ \mathbf{a}^* = -\mathbf{a}/2, \mathbf{b}^* = \mathbf{c}/2 \]
Origin at 0,y,0
Aba21'  mm21'  Orthorhombic
41.2.301  Aba21'

Origin on 11n21'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1  
(2) 2  0,0,z  
(3) a  (1/2,0,0)  x,1/4,z  
(4) b  (0,1/2,0)  1/4,y,z

(1* 0,0,0)  
(2* 0,0,0)  
(3* 1/2,1/2,0)  
(4* 1/2,1/2,0)

For (0,1/2,1/2) + set

(1) t  (0,1/2,1/2)  
(2) 2  (0,0,1/2)  0,1/4,z  
(3) n  (1/2,0,1/2)  x,0,z  
(4) c  (0,0,1/2)  1/4,y,z

(1* 0,1/2,1/2)  
(2* 0,1/2,1/2)  
(3* 1/2,0,1/2)  
(4* 1/2,0,1/2)

For (0,0,0)' + set

(1) 1'  
(2) 2'  0,0,z  
(3) a'  (1/2,0,0)  x,1/4,z  
(4) b'  (0,1/2,0)  1/4,y,z

(1* 0,0,0)'  
(2* 0,0,0)'  
(3* 1/2,1/2,0)'  
(4* 1/2,1/2,0)'

For (0,1/2,1/2) + set

(1) t'  (0,1/2,1/2)  
(2) 2'  (0,0,1/2)  0,1/4,z  
(3) n'  (1/2,0,1/2)  x,0,z  
(4) c'  (0,0,1/2)  1/4,y,z

(1* 0,1/2,1/2)  
(2* 0,1/2,1/2)'  
(3* 1/2,0,1/2)  
(4* 1/2,0,1/2)'


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Generators selected (1): t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); 1'.

Positions

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<td>(0,0,0)' +</td>
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<td>(0,1/2,1/2) +</td>
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<tr>
<td>8 b 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 a .21'</td>
<td>(3) x+1/2,y+1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 a .21'</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg1'  
\[ a^* = a \quad b^* = b/2 \]
Origin at 0,0,z

Along [1,0,0] p1m11'  
\[ a^* = b/2 \quad b^* = c/2 \]
Origin at x,0,0

Along [0,1,0] p1m11'  
\[ a^* = -a/2 \quad b^* = c/2 \]
Origin at 0,y,0
Orthorhombic

Ab’a2' m’m2'

41.3.302 Ab’a2'

**Origin** on 1n2'

**Asymmetric unit**

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

**Symmetry Operations**

**For (0,0,0) + set**

1. \( (1) 1 \)
   
   \[ (1 | 0,0,0) \]

2. \( (2) 2' \quad 0,0,z \)
   
   \[ (2 | 0,0,0)' \]

3. \( (3) a \quad (1/2,0,0) \)
   
   \[ x,1/4,z \quad (m | 1/2,1/2,0) \]

4. \( (4) b' \quad (0,1/2,0) \)
   
   \[ 1/4,y,z \quad (m | 1/2,1/2,0)' \]

**For (0,1/2,1/2) + set**

1. \( (1) t \quad (0,1/2,1/2) \)
   
   \[ (1 | 0,1/2,1/2) \]

2. \( (2) 2' \quad (0,0,1/2) \)
   
   \[ 0,1/4,z \quad (2 | 0,1/2,1/2)' \]

3. \( (3) n \quad (1/2,0,1/2) \)
   
   \[ x,0,z \quad (m | 1/2,0,1/2) \]

4. \( (4) c' \quad (0,0,1/2) \)
   
   \[ 1/4,y,z \quad (m | 1/2,0,1/2)' \]
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>8 b 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 a ..2' 0,0,z [u,v,0] 1/2,1/2,z [u,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p2'm'g
  - \( a^* = a \quad b^* = b/2 \)
  - Origin at 0,0,z

- Along [1,0,0] p1m1
  - \( a^* = b/2 \quad b^* = c/2 \)
  - Origin at x,0,0

- Along [0,1,0] p2a1m1
  - \( a^* = -a/2 \quad b^* = c/2 \)
  - Origin at 0,y,0
Origin on 1n'2'

Asymmetric unit  \(0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}\)

Symmetry Operations

For \((0,0,0) + \) set

(1) 1  
   (1 | 0,0,0)

(2) 2' 0,0,z  
   \((2_z | 0,0,0)\)‘

(3) a' (1/2,0,0)  x,1/4,z  
   \((m_y | 1/2,1/2,0)\)‘

(4) b (0,1/2,0)  1/4,y,z  
   \((m_x | 1/2,1/2,0)\)

For \((0,1/2,1/2) + \) set

(1) t (0,1/2,1/2)  
   \((1 | 0,1/2,1/2)\)

(2) 2' (0,0,1/2)  0,1/4,z  
   \((2_z | 0,1/2,1/2)\)‘

(3) n' (1/2,0,1/2)  x,0,z  
   \((m_y | 1/2,0,1/2)\)‘

(4) c (0,0,1/2)  1/4,y,z  
   \((m_x | 1/2,0,1/2)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1)</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>0,0,z [u,v,0]</td>
<td>(2)</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2'mg'
  - $a^* = a$, $b^* = b/2$
  - Origin at 0,0,z
- Along [1,0,0] p$_{2a*}$1m1
  - $a^* = b/2$, $b^* = c/2$
  - Origin at x,0,0
- Along [0,1,0] p1m1
  - $a^* = -a/2$, $b^* = c/2$
  - Origin at 0,y,0
Ab'a'2
41.5.304

m'm'2
Ab'a'2

Orthorhombic

Origin on 1n'2

Asymmetric unit:
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set:

(1) 1
   (1) 0,0,0

(2) 2 0,0,z
(2) x,1/4,z
(2) 0,0,0)
(2) x,0,z

(3) a' (1/2,0,0) x,1/4,z
(3) a (1/2,0,0) x,1/4,z
(3) (m_y|1/2,1/2,0)

(4) b' (0,1/2,0) 1/4,y,z
(4) b (0,1/2,0) 1/4,y,z
(4) (m_x|1/2,1/2,0)

For (0,1/2,1/2) + set:

(1) t (0,1/2,1/2)
(1) 0,1/2,1/2

(2) 2 0,0,1/2 0,1/4,z
(2) x,0,1/2 0,1/4,z
(2) (m_y|1/2,1/2,0)

(3) n' (1/2,0,1/2) x,0,z
(3) n (1/2,0,1/2) x,0,z
(3) (m_x|1/2,1/2,0)

(4) c' (0,0,1/2) 1/4,y,z
(4) c (0,0,1/2) 1/4,y,z
(4) (m_x|1/2,1/2,0)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 a 2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'g'  
Along [1,0,0] p1m'1  
Along [0,1,0] p1m'1

\( a^* = a \quad b^* = b/2 \)  
\( a^* = b/2 \quad b^* = c/2 \)  
\( a^* = -a/2 \quad b^* = c/2 \)

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
41.6.305 - 1 - 586

**Origin** on 1n'2

**Asymmetric unit**

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \]

**Symmetry Operations**

For (0,0,0) + set

1. \(1\)
   
   \((1) \begin{cases} 1 \\ (1|0,0,0) \end{cases}\)

2. \(2\)
   
   \((2) \begin{cases} 2 \quad 0,0,z \\ (2|0,0,0) \end{cases}\)

3. \(a\)
   
   \((3) \begin{cases} a \quad (1/2,0,0) \quad x,1/4,z \\ (m,|1/2,1/2,0) \end{cases}\)

4. \(b\)
   
   \((4) \begin{cases} b \quad (0,1/2,0) \quad 1/4,y,z \\ (m,|1/2,1/2,0) \end{cases}\)

For (0,1/2,1/2)' + set

1. \(t'\)
   
   \((1) t' \begin{cases} (0,1/2,1/2) \\ (1|0,1/2,1/2)' \end{cases}\)

2. \(2'\)
   
   \((2) 2' \begin{cases} (0,0,1/2) \quad 0,1/4,z \\ (2|0,1/2,1/2)' \end{cases}\)

3. \(n'\)
   
   \((3) n' \begin{cases} (1/2,0,1/2) \quad x,0,z \\ (m,|1/2,0,1/2)' \end{cases}\)

4. \(c'\)
   
   \((4) c' \begin{cases} (0,0,1/2) \quad 1/4,y,z \\ (m,|1/2,0,1/2)' \end{cases}\)
Generators selected  (1); \( t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); (2); (3). \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) ( x,y,z \ [u,v,w] ) ( (0,0,0) ) + ( (0,1/2,1/2)' ) + ( (0,1/2,1/2) )</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w] ( 1/2,1/2,z \ [u,v,w] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] ( p_{2a}.2m'g' )</th>
<th>Along [1,0,0] ( p_{2a}.1m1 )</th>
<th>Along [0,1,0] ( p_{c}.1m1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) ( b^* = b/2 )</td>
<td>( a^* = b/2 ) ( b^* = c/2 )</td>
<td>( a^* = -a/2 ) ( b^* = c/2 )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin on 1n'2'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set
(1) 1
   (1 | 0,0,0)
(2) 2' 0,0,z
   (2 | 0,0,0)'
(3) a (1/2,0,0) x,1/4,z
   (m | 1/2,1/2,0)
(4) b' (0,1/2,0) 1/4,y,z
   (m | 1/2,1/2,0)'

For (0,1/2,1/2)' + set
(1) t' (0,1/2,1/2)
   (1 | 0,1/2,1/2)'
(2) 2 (0,0,1/2) 0,1/4,z
   (2 | 0,1/2,1/2)
(3) n' (1/2,0,1/2) x,0,z
   (m | 1/2,0,1/2)'
(4) c (0,0,1/2) 1/4,y,z
   (m | 1/2,0,1/2)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [u,v,w]</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{2a} \cdot 2mg \)  
Along [1,0,0] \( p_{2a} \cdot 1m1 \)  
Along [0,1,0] \( p_c \cdot 1m1 \)

\( a^* = a \)  \( b^* = b/2 \)  
Origin at 0,1/4,z  
\( a^* = b/2 \)  \( b^* = c/2 \)  
Origin at x,0,0  
\( a^* = -a/2 \)  \( b^* = c/2 \)  
Origin at 0,y,0
Origin on 1n2'

Asymmetric unit  
$0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1  \hspace{1cm} (2) 2' 0,0,z  \hspace{1cm} (3) a' (1/2,0,0) x,1/4,z  \hspace{1cm} (4) b (0,1/2,0) 1/4,y,z

(1*) 0,0,0  \hspace{1cm} (2*) 0,0,0'  \hspace{1cm} (3*) (1/2,1/2,0)' \hspace{1cm} (4*) (1/2,1/2,0)

For $(0,1/2,1/2)' +$ set

(1) t' (0,1/2,1/2)  \hspace{1cm} (2) 2 (0,1/2,1/2) 0,1/4,z  \hspace{1cm} (3) n (1/2,0,1/2) x,0,z  \hspace{1cm} (4) c' (0,0,1/2) 1/4,y,z

(1*) (0,1/2,1/2)'  \hspace{1cm} (2*) (0,1/2,1/2)  \hspace{1cm} (3*) (1/2,0,1/2) \hspace{1cm} (4*) (1/2,0,1/2)'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); (2); (3).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2)' +</td>
</tr>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x' y',z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2, y+1/2, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2, y+1/2, z' [u,v,w]</td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2, z' [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]    p2a.2m'g'    a* = a    b* = b/2    Origin at 0,1/4,z
Along [1,0,0]    p2a.1m1      a* = b/2    b* = c/2    Origin at x,0,0
Along [0,1,0]    p2a.1m1      a* = -a/2    b* = c/2    Origin at 0,y,0
Origin on 1n2

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1 (0,0,0)$
2. $2 (0,0,z)$
3. $a' (1/2,0,0) x,1/4,z$
4. $b' (0,1/2,0) 1/4,y,z$

For $(0,1/2,1/2)' +$ set

1. $t' (0,1/2,1/2)$
2. $2' (0,0,1/2) 0,1/4,z$
3. $n (1/2,0,1/2) x,0,z$
4. $c (0,0,1/2) 1/4,y,z$

$A_p b'a'2 \quad mm21' \quad Orthorhombic$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); (2); (3).

Positions  

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2)’ +</td>
<td></td>
</tr>
<tr>
<td>8 b 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x+1/2,y+1/2,z [u,v,w] (4) x+1/2,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 a ..2 0,0,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2g-2mg</th>
<th>Along [1,0,0] p2g-1m1</th>
<th>Along [0,1,0] p2g-1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a  b* = b/2</td>
<td>a* = b/2  b* = c/2</td>
<td>a* = -a/2  b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Fmm2 mm2 Orthorhombic
42.1.309 Fmm2

Origin on mm2

Asymmetric unit

\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 0,0,z \\
(3) & \quad m \ x,0,z \\
(4) & \quad m \ 0,y,z
\end{align*}
\]

\[
\begin{align*}
(1^*) & \quad 0,0,0 \\
(2^*) & \quad 0,0,0 \\
(3^*) & \quad 0,0,0 \\
(4^*) & \quad 0,0,0
\end{align*}
\]

For \((0,1/2,1/2) + \) set

\[
\begin{align*}
(1) & \quad t \ (0,1/2,1/2) \\
(2) & \quad 2 \ (0,0,1/2) \ 0,1/4,z \\
(3) & \quad c \ (0,0,1/2) \ x,1/4,z \\
(4) & \quad n \ (0,1/2,1/2) \ 0,y,z
\end{align*}
\]

\[
\begin{align*}
(1^*) & \quad 0,1/2,1/2 \\
(2^*) & \quad 0,1/2,1/2 \\
(3^*) & \quad 0,1/2,1/2 \\
(4^*) & \quad 0,1/2,1/2
\end{align*}
\]

For \((1/2,0,1/2) + \) set

\[
\begin{align*}
(1) & \quad t \ (1/2,0,1/2) \\
(2) & \quad 2 \ (0,0,1/2) \ 1/4,0,z \\
(3) & \quad n \ (1/2,0,1/2) \ x,0,z \\
(4) & \quad c \ (0,0,1/2) \ 1/4,y,z
\end{align*}
\]

\[
\begin{align*}
(1^*) & \quad 1/2,0,1/2 \\
(2^*) & \quad 1/2,0,1/2 \\
(3^*) & \quad 1/2,0,1/2 \\
(4^*) & \quad 1/2,0,1/2
\end{align*}
\]

For \((1/2,1/2,0) + \) set

\[
\begin{align*}
(1) & \quad t \ (1/2,1/2,0) \\
(2) & \quad 2 \ 1/4,1/4,z \\
(3) & \quad a \ (1/2,1/2,0) \ x,1/4,z \\
(4) & \quad b \ (0,1/2,0) \ 1/4,y,z
\end{align*}
\]

\[
\begin{align*}
(1^*) & \quad 1/2,1/2,0 \\
(2^*) & \quad 1/2,1/2,0 \\
(3^*) & \quad 1/2,1/2,0 \\
(4^*) & \quad 1/2,1/2,0
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>16 e</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(0,1/2,1/2)</td>
<td>8 d.m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>(1/2,0,1/2)</td>
<td>8 c.m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>(1/2,1/2,0)</td>
<td>8 b..2</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>(0,0,0)</td>
<td>4 a mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm

<table>
<thead>
<tr>
<th>a* = a/2</th>
<th>b* = b/2</th>
</tr>
</thead>
</table>

Origin at 0,0,z

Along [1,0,0] p1m11'

<table>
<thead>
<tr>
<th>a* = b/2</th>
<th>b* = c/2</th>
</tr>
</thead>
</table>

Origin at x,0,0

Along [0,1,0] p1m11'

<table>
<thead>
<tr>
<th>a* = -a/2</th>
<th>b* = c/2</th>
</tr>
</thead>
</table>

Origin at 0,y,0
Origin on mm21'  
Asymmetric unit  
\[0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1\]

Symmetry Operations

For (0,0,0) + set

1. \(1\)  
2. \(2\) \(0,0,z\)  
3. \(m\) \(x,0,z\)  
4. \(m\) \(0,y,z\)

For (0,1/2,1/2) + set

1. \(t\) \((0,1/2,1/2)\)  
2. \(2\) \(0,1/2,1/2\) \(0,1/4,z\)  
3. \(c\) \((0,0,1/2)\) \(x,1/4,z\)  
4. \(n\) \((0,1/2,1/2)\) \(0,y,z\)

For (1,2,1/2) + set

1. \(t\) \((1/2,0,1/2)\)  
2. \(2\) \((0,0,1/2)\) \(1/4,0,z\)  
3. \(n\) \((1/2,0,1/2)\) \(x,0,z\)  
4. \(c\) \((0,0,1/2)\) \(1/4,y,z\)

For (0,0,0)' + set

1. \(1'\)  
2. \(2'\) \(0,0,z\)  
3. \(m'\) \(x,0,z\)  
4. \(m'\) \(0,y,z\)

For (0,1/2,1/2)' + set

1. \(t'\) \((0,1/2,1/2)\)  
2. \(2'\) \((0,0,1/2)\) \(0,1/4,z\)  
3. \(c'\) \((0,0,1/2)\) \(x,1/4,z\)  
4. \(n'\) \((0,1/2,1/2)\) \(0,y,z\)
Continued

For $(1/2,0,1/2)' + \text{set}$

$(1) \ t' (1/2,0,1/2)$
$(1) |(1/2,0,1/2)'$

$(2) \ 2' (0,0,1/2) \ 1/4,0,z$
$(2) |(1/2,0,1/2)'$

$(3) \ n' (1/2,0,1/2) \ x,0,z$
$(m, |1/2,0,1/2)'$

$(4) \ c' (0,0,1/2) \ 1/4,y,z$
$(m, |1/2,0,1/2)'$

For $(1/2,1/2,0)' + \text{set}$

$(1) \ t' (1/2,1/2,0)$
$(1) |(1/2,1/2,0)'$

$(2) \ 2' 1/4,1/4,z$
$(2) |(1/2,1/2,0)'$

$(3) \ a' (1/2,0,0) \ x,1/4,z$
$(m, |1/2,1/2,0)'$

$(4) \ b' (0,1/2,0) \ 1/4,y,z$
$(m, |1/2,1/2,0)'$

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

$(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +$

$(0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)' +$

16 e 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]

8 d .m.1' x,0,z [0,0,0] x,0,z [0,0,0]

8 c m..1' 0,y,z [0,0,0] 0,y,z [0,0,0]

8 b ..21' 1/4,1/4,z [0,0,0] 1/4,3/4,z [0,0,0]

4 a mm21' 0,0,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2mm1'  Along [1,0,0] p1m11'  Along [0,1,0] p1m11'

$a^* = a/2$  $b^* = b/2$  $a^* = b/2$  $b^* = c/2$

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0

42.2.310 - 2 - 597
Fm'\text{m}2' \quad \text{m}'\text{m}2' \quad \text{Orthorhombic}

42.3.311

Origin on m'\text{m}2'

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) $1$
(1 $|0,0,0)$

(2) $2'$ $0,0,z$
(2 $|0,0,0)'$

(3) $m$ $x,0,z$
(m $|0,0,0)$

(4) $m'$ $0,y,z$
(m $|0,0,0)'$

For (0,1/2,1/2) + set

(1) $t$ (0,1/2,1/2)$
(1 $|1/2,0,1/2)$

(2) $2'$ (0,0,1/2) $1/4,0,z$
(2 $|0,1/2,0,1/2)'$

(3) $c$ (0,0,1/2) $x,1/4,z$
(m $|0,1/2,1/2)$

(4) $n'$ (0,1/2,1/2) $0,y,z$
(m $|0,1/2,1/2)'$

For (1/2,0,1/2) + set

(1) $t$ (1/2,0,1/2)$
(1 $|1/2,0,0,1/2)$

(2) $2'$ (0,0,1/2) $1/4,0,z$
(2 $|1/2,0,0,1/2)'$

(3) $n$ (1/2,0,1/2) $x,0,z$
(m $|1/2,0,1/2)$

(4) $c'$ (0,0,1/2) $1/4,y,z$
(m $|1/2,0,1/2)'$

For (1/2,1/2,0) + set

(1) $t$ (1/2,1/2,0)$
(1 $|1/2,1/2,0)$

(2) $2'$ $1/4,1/4,z$
(2 $|1/2,1/2,0)'$

(3) $a$ (1/2,0,0) $x,1/4,z$
(m $|1/2,1/2,0)$

(4) $b'$ (0,1/2,0) $1/4,y,z$
(m $|1/2,1/2,0)'$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>16 e 1 x,y,z[u,v,w] (2) x,y,z[u,v,w] (3) x,y,z[ū,v,w] (4) x,y,z[ū,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 d m. x,0,z[0,v,0] x,0,z[0,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 c m'. 0,y,z[0,v,w] 0,y,z[0,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 b .2' 1/4,1/4,z[u,v,0] 1/4,3/4,z[ū,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 a m'2' 0,0,z[0,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mmm'  
\( \mathbf{a}^* = -\mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{a}/2 \)  
Origin at 0,0,z

Along [1,0,0] p1m1  
\( \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at x,0,0

Along [0,1,0] p1m11'  
\( \mathbf{a}^* = -\mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at 0,y,0
Orthorhombic

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1 \]

Symmetry Operations

For \((0,0,0)\) + set

1. \(E\) \((0,0,0)\)
2. \((2)\) \((0,0,z)\)
3. \((3)\) \(x,0,z\)
4. \((4)\) \(0,y,z\)

For \((0,1/2,1/2)\) + set

1. \(t\) \((0,1/2,1/2)\)
2. \((2)\) \((0,0,1/2)\)
3. \((3)\) \(0,1/4,z\)
4. \((4)\) \(0,1/4,z\)

For \((1/2,0,1/2)\) + set

1. \(t\) \((1/2,0,1/2)\)
2. \((2)\) \((0,1/2,0)\)
3. \((3)\) \(1/4,0,z\)
4. \((4)\) \(1/4,0,z\)

For \((1/2,1/2,0)\) + set

1. \(t\) \((1/2,1/2,0)\)
2. \((2)\) \((1/4,1/4,z)\)
3. \((3)\) \(1/4,1/4,z\)
4. \((4)\) \(1/4,1/4,z\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity,</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>16 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 d .m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>8 c m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 b .2</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>4 a m'm'2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  p2m'm'  
**a** = a/2  **b** = b/2  
Origin at 0,0,z

Along [1,0,0]  p1m'1  
**a** = b/2  **b** = c/2  
Origin at x,0,0

Along [0,1,0]  p1m'1  
**a** = -a/2  **b** = c/2  
Origin at 0,y,0
**Symmetry Operations**

For (0,0,0) + set

1. 1
2. 2 \(0,0,z\)
3. \(m\) \(x,0,z\)
4. \(m\) \(0,y,z\)

For (0,1/2,1/2)' + set

1. \(t\) \((0,1/2,1/2)\)
2. \(2'\) \((0,0,1/2)\)
3. \(c'\) \((0,0,1/2)\)
4. \(n'\) \((0,1/2,1/2)\)

For (1/2,0,1/2)' + set

1. \(t\) \((1/2,0,1/2)\)
2. \(2'\) \((0,0,1/2)\)
3. \(n'\) \((1/2,0,1/2)\)
4. \(c'\) \((0,0,1/2)\)

For (1/2,1/2,0) + set

1. \(t\) \((1/2,1/2,0)\)
2. \(2\) \(1/4,1/4,z\)
3. \(a\) \((1/2,0,0)\)
4. \(b\) \((0,1/2,0)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

Positions

Multiplicity,  Wyckoff letter,  Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2)' +</td>
<td>(1/2,0,1/2)' +</td>
</tr>
<tr>
<td>16 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 d .m.</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 c m..</td>
<td>0,y,z [0,v,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 a mm2</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p-2mm  Along [1,0,0]  p1m11'  Along [0,1,0]  p1m11'
\( \mathbf{a}^* = \mathbf{a}/2 \)  \( \mathbf{b}^* = \mathbf{b}/2 \)  \( \mathbf{a}^* = -\mathbf{a}/2 \)  \( \mathbf{b}^* = \mathbf{c}/2 \)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin on mm2

Asymmetric unit $0 \leq x \leq 1/4$; $0 \leq y \leq 1/4$; $0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
   
   (1) 1
   (2) 2 0,0,0
   (3) $m$ x,0,0
   (4) $m$ 0,y,z

   For $(0,1/2,1/2) +$ set

1. $t$ (0,1/2,1/2)
   
   (1) $t$ (0,1/2,1/2)
   (2) 2 (0,0,1/2) 0,1/4,0
   (3) $c$ (0,0,1/2) x,1/4,0
   (4) $n$ (0,1/2,1/2) 0,y,z

   For $(1/2,0,1/2)' +$ set

1. $t'$ (1/2,0,1/2)
   
   (1) $t'$ (1/2,0,1/2)
   (2) 2' (0,0,1/2) 1/4,0,0
   (3) $n'$ (1/2,0,1/2) x,0,0
   (4) $c'$ (0,0,1/2) 1/4,y,z

   For $(1/2,1/2,0)' +$ set

1. $b'$ (1/2,1/2,0)
   
   (1) $b'$ (1/2,1/2,0)
   (2) 2' 1/4,1/4,0
   (3) $a'$ (1/2,0,0) x,1/4,0
   (4) $b'$ (0,1/2,0) 1/4,y,z
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(x,y,z) [u,v,w]</td>
</tr>
<tr>
<td>(0,1/2,1/2) +</td>
<td>(\bar{x},0,z) [0,v,0]</td>
</tr>
<tr>
<td>(1/2,0,1/2)' +</td>
<td>(x,y,z) [(\bar{u},v,\bar{w})]</td>
</tr>
<tr>
<td>(1/2,1/2,0)' +</td>
<td>(x,y,z) [u,v,(\bar{w})]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\)  \(p_{2a}2mm\)  \(p_{2a}2mm\)  \(p_{2a}2mm\)
\(a^*=a/2\)  \(b^*=b/2\)  \(a^*=a/2\)  \(b^*=b/2\)
Origin at \(0,0,z\)  Origin at \(x,0,0\)  Origin at \(0,y,0\)  Origin at \(0,y,0\)
42.7.315 - 1 - 606

**Orthorhombic**

- **Origin**: on mm'2'
- **Asymmetric unit**: $0 < x < 1/4; 0 < y < 1/4; 0 < z < 1$

**Symmetry Operations**

For $(0,0,0) +$ set

1. $1$
   
2. $2' \ (0,0,z)$
   
3. $m' \ x,0,z$
   
4. $m \ 0,y,z$

For $(0,1/2,1/2)' +$ set

1. $t' \ (0,1/2,1/2)$
   
2. $2 \ (0,0,1/2) \ 0,1/4,z$
   
3. $c \ (0,0,1/2) \ x,1/4,z$
   
4. $n' \ (0,1/2,1/2) \ 0,y,z$

For $(1/2,0,1/2)' +$ set

1. $t' \ (1/2,0,1/2)$
   
2. $2 \ (0,0,1/2) \ 1/4,0,z$
   
3. $n \ (1/2,0,1/2) \ x,0,z$
   
4. $c' \ (0,0,1/2) \ 1/4,y,z$

For $(1/2,1/2,0) +$ set

1. $t \ (1/2,1/2,0)$
   
2. $2' \ 1/4,1/4,z$
   
3. $a' \ (1/2,0,0) \ x,1/4,z$
   
4. $b \ (0,1/2,0) \ 1/4,y,z$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

Positions

<table>
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<tr>
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<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>16 e 1 (1) x,y,z [u,v,w]</td>
<td>(2) \overline{x},y,z [u,v,w]</td>
</tr>
<tr>
<td>8 d .m'. x,0,z [u,0,w]</td>
<td>\overline{x},0,z [u,0,w]</td>
</tr>
<tr>
<td>8 c m.. 0,y,z [u,0,0]</td>
<td>0,\overline{y},z [u,0,0]</td>
</tr>
<tr>
<td>8 b ..2' 1/4,1/4,z [u,v,0]</td>
<td>1/4,3/4,z [u,\overline{v},0]</td>
</tr>
<tr>
<td>4 a mm'2' 0,0,z [u,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm  
\(a^* = a/2\)  \(b^* = b/2\)
Origin at 0,1/4,z

Along [1,0,0] p1m11'  
\(a^* = b/2\)  \(b^* = c/2\)
Origin at 0,0,0

Along [0,1,0] p2\(1\overline{m}1\)  
\(a^* = -a/2\)  \(b^* = c/2\)
Origin at 0,y,0
Origin on \( m'm2 \)

Asymmetric unit \( 0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 0,0,z \\
(3) & \quad m', x,0,z \\
(4) & \quad m', 0,y,z \\
(1') & \quad 0,0,0 \\
(2') & \quad 0,0,0' \\
(3') & \quad m', 0,0,0' \\
(4') & \quad m', 0,0,0'
\end{align*}
\]

For \((0,1/2,1/2) + \) set

\[
\begin{align*}
(1) & \quad t' (0,1/2,1/2) \\
(2) & \quad 2', 0,0,1/2,1/2 \\
(3) & \quad c, 0,0,1/2 \\
(4) & \quad n, 0,1/2,1/2,1/2 \\
(1') & \quad 0,1/2,1/2 \\
(2') & \quad 0,0,0 \\
(3') & \quad m, 0,0,1/2,1/2 \\
(4') & \quad m, 0,1/2,1/2,1/2
\end{align*}
\]

For \((1/2,0,1/2) + \) set

\[
\begin{align*}
(1) & \quad t' (1/2,0,1/2) \\
(2) & \quad 2', 0,0,1/2,1/2 \\
(3) & \quad n, 1/2,0,1/2,1/2 \\
(4) & \quad c, 0,0,1/2 \\
(1') & \quad 1/2,0,1/2 \\
(2') & \quad 0,0,0 \\
(3') & \quad m, 0,0,1/2,1/2 \\
(4') & \quad m, 0,1/2,1/2,1/2
\end{align*}
\]

For \((1/2,1/2,0) + \) set

\[
\begin{align*}
(1) & \quad t (1/2,1/2,0) \\
(2) & \quad 2, 1/4,1/4,z \\
(3) & \quad a', 1/2,0,0 \\
(4) & \quad b', 0,1/2,0 \\
(1') & \quad 1/2,1/2,0 \\
(2') & \quad 1/2,1/2,0 \\
(3') & \quad m, 1/2,1/2,0 \\
(4') & \quad m, 1/2,1/2,0'
\end{align*}
\]
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3). \)

**Positions**

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<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 e 1</td>
<td>(1) (x,y,z) [(u,v,w)]</td>
</tr>
<tr>
<td>8 d m'</td>
<td>(2) (\bar{x},y,z) [(\bar{u},v,w)]</td>
</tr>
<tr>
<td>8 c m'</td>
<td>(3) (x,\bar{y},z) [(u,\bar{v},w)]</td>
</tr>
<tr>
<td>8 b ..2</td>
<td>(4) (\bar{x},y,z) [(\bar{u},v,w)]</td>
</tr>
<tr>
<td>4 a m'm'2</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along \([0,0,1]\) \(\text{p}_{\text{c}2\text{mm}}\)
\(a^*=\frac{a}{2} \quad b^*=\frac{b}{2}\)
Origin at 1/4,1/4,z

Along [1,0,0] \(\text{p}_{2\text{b}1\text{m}1}\)
\(a^*=\frac{b}{2} \quad b^*=\frac{c}{2}\)
Origin at \(x,0,0\)

Along [0,1,0] \(\text{p}_{2\text{b}1\text{m}1}\)
\(a^*=\frac{-a}{2} \quad b^*=\frac{c}{2}\)
Origin at 0,y,0
Origin on m'm2'

Asymmetric unit \(0 < x < 1/4; \quad 0 < y < 1/4; \quad 0 < z < 1\)

Symmetry Operations

For \((0,0,0) + \) set

(1) \(1\)
(2) \(2' \quad 0,0,z\)
(3) \(m \quad x,0,z\)
(4) \(m' \quad 0,y,z\)

For \((0,1/2,1/2) + \) set

(1) \(t \quad (0,1/2,1/2)\)
(2) \(2' \quad (0,0,1/2) \quad 0,1/4,z\)
(3) \(c \quad (0,0,1/2) \quad x,1/4,z\)
(4) \(n' \quad (0,1/2,1/2) \quad 0,y,z\)

For \((1/2,0,1/2) + \) set

(1) \(t' \quad (1/2,0,1/2)\)
(2) \(2 \quad (0,0,1/2) \quad 1/4,0,z\)
(3) \(n' \quad (1/2,0,1/2) \quad x,0,z\)
(4) \(c \quad (0,0,1/2) \quad 1/4,y,z\)

For \((1/2,1/2,0) + \) set

(1) \(t' \quad (1/2,1/2,0)\)
(2) \(2 \quad 1/4,1/4,z\)
(3) \(a' \quad (1/2,0,0) \quad x,1/4,z\)
(4) \(b \quad (0,1/2,0) \quad 1/4,y,z\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2)' + (1/2,1/2,0)' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 d m..</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 c m'..</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 b ..2'</td>
<td>1/4,1/4,z [u,v,0]</td>
<td>1/4,3/4,z [u,v,0]</td>
</tr>
<tr>
<td>4 a m'm2'</td>
<td>0,0,z [0,v,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,1,0] p2a*2mm
\[ a^* = a/2 \quad b^* = b/2 \]
Origin at 0,1/4,z

Along [1,0,0] p..1m1
\[ a^* = b/2 \quad b^* = c/2 \]
Origin at x,0,0

Along [0,1,0] p1m11'
\[ a^* = -a/2 \quad b^* = c/2 \]
Origin at 0,y,0
Origin on mm'2'

Asymmetric unit \( 0 < x < 1/4; \quad 0 < y < 1/4; \quad 0 < z < 1 \)

Symmetry Operations

For \((0,0,0) + \) set

1. \((0,0,0)\)
2. \((0,0,0)', \quad (0,0,0)\)
3. \((0,0,0)', \quad (0,0,0)\)
4. \((0,0,0)', \quad (0,0,0)\)

For \((0,1/2,1/2) + \) set

1. \((0,1/2,1/2)\)
2. \((0,1/2,1/2)', \quad (0,1/2,1/2)\)
3. \((0,1/2,1/2)', \quad (0,1/2,1/2)\)
4. \((0,1/2,1/2)', \quad (0,1/2,1/2)\)

For \((1/2,0,1/2) + \) set

1. \((1/2,0,1/2)\)
2. \((1/2,0,1/2)', \quad (1/2,0,1/2)\)
3. \((1/2,0,1/2)', \quad (1/2,0,1/2)\)
4. \((1/2,0,1/2)', \quad (1/2,0,1/2)\)

For \((1/2,1/2,0) + \) set

1. \((1/2,1/2,0)\)
2. \((1/2,1/2,0)', \quad (1/2,1/2,0)\)
3. \((1/2,1/2,0)', \quad (1/2,1/2,0)\)
4. \((1/2,1/2,0)', \quad (1/2,1/2,0)\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Sites</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>16 e</td>
</tr>
<tr>
<td>(0,1/2,1/2)</td>
<td>8 d</td>
</tr>
<tr>
<td>(1/2,0,1/2)'</td>
<td>8 c</td>
</tr>
<tr>
<td>(1/2,1/2,0)'</td>
<td>8 b</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a'}2m'm'
\[ a^* = a/2 \quad b^* = b/2 \]
Origin at 1/4,0,z

Along [1,0,0] p_{1m11'}
\[ a^* = b/2 \quad b^* = c/2 \]
Origin at x,0,0

Along [0,1,0] p_{2a',1m1}
\[ a^* = -a/2 \quad b^* = c/2 \]
Origin at 0,y,0
Origin on \( m'm'2 \)

Asymmetric unit \( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
&\text{(1) } \begin{pmatrix} 1 \end{pmatrix} \\
&\text{(2) } \begin{pmatrix} 2 \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} \\
&\text{(3) } \begin{pmatrix} m' \end{pmatrix} \begin{pmatrix} x,0,z \end{pmatrix} \\
&\text{(4) } \begin{pmatrix} m' \end{pmatrix} \begin{pmatrix} 0,y,z \end{pmatrix}
\end{align*}
\]

For \((0,1/2,1/2)\) + set

\[
\begin{align*}
&\text{(1) } \begin{pmatrix} t \end{pmatrix} \begin{pmatrix} 0,1/2,1/2 \end{pmatrix} \\
&\text{(2) } \begin{pmatrix} 2 \end{pmatrix} \begin{pmatrix} 0,0,1/2 \end{pmatrix} \begin{pmatrix} 0,1/4,z \end{pmatrix} \\
&\text{(3) } \begin{pmatrix} c' \end{pmatrix} \begin{pmatrix} 0,0,1/2 \end{pmatrix} \begin{pmatrix} x,1/4,z \end{pmatrix} \\
&\text{(4) } \begin{pmatrix} n' \end{pmatrix} \begin{pmatrix} 0,1/2,1/2 \end{pmatrix} \begin{pmatrix} 0,y,z \end{pmatrix} \\
&\text{(5) } \begin{pmatrix} m' \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix}' \begin{pmatrix} m_x \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix}'
\end{align*}
\]

For \((1/2,0,1/2)'\) + set

\[
\begin{align*}
&\text{(1) } \begin{pmatrix} t' \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix} \\
&\text{(2) } \begin{pmatrix} 2' \end{pmatrix} \begin{pmatrix} 0,0,1/2 \end{pmatrix} \begin{pmatrix} 1/4,0,z \end{pmatrix} \\
&\text{(3) } \begin{pmatrix} n \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix} \begin{pmatrix} x,0,z \end{pmatrix} \\
&\text{(4) } \begin{pmatrix} c \end{pmatrix} \begin{pmatrix} 0,0,1/2 \end{pmatrix} \begin{pmatrix} 1/4,y,z \end{pmatrix} \\
&\text{(5) } \begin{pmatrix} m \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix} \begin{pmatrix} m_x \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix}
\end{align*}
\]

For \((1/2,1/2,0)' + set\)

\[
\begin{align*}
&\text{(1) } \begin{pmatrix} t' \end{pmatrix} \begin{pmatrix} 1/2,1/2,0 \end{pmatrix} \\
&\text{(2) } \begin{pmatrix} 2' \end{pmatrix} \begin{pmatrix} 1/4,1/4,0 \end{pmatrix} \begin{pmatrix} 1/4,z \end{pmatrix} \\
&\text{(3) } \begin{pmatrix} a \end{pmatrix} \begin{pmatrix} 1/2,0,0 \end{pmatrix} \begin{pmatrix} x,1/4,z \end{pmatrix} \\
&\text{(4) } \begin{pmatrix} b \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} 1/4,y,z \end{pmatrix} \\
&\text{(5) } \begin{pmatrix} m \end{pmatrix} \begin{pmatrix} 1/2,1/2,0 \end{pmatrix} \begin{pmatrix} m_x \end{pmatrix} \begin{pmatrix} 1/2,1/2,0 \end{pmatrix}
\end{align*}
\]
Generators selected

(1); t/(1,0,0); t(0,0,1); t(0,1,0); t(0,1/2,1/2); t'(1/2,0,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2)’ + (1/2,1/2,0)’ +</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 e 1</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 d m’</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 c m’</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 b m’2</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>4 a m’2</td>
<td>0,y,z [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a2m’m’

a* = a/2  b* = b/2
Origin at 0,0,z

Along [1,0,0] p,,1m1

a* = b/2  b* = c/2
Origin at x,1/4,0

Along [0,1,0] p2a1m1

a* = -a/2  b* = c/2
Origin at 1/4,y,0
Origin on 112

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z
(3) d (1/4,0,1/4) x,1/8,z
(4) d (0,1/4,1/4) 1/8,y,z

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)
(2) 2 (0,0,1/2) 0,1/4,z
(3) d (1/4,0,3/4) x,3/8,z
(4) d (0,3/4,3/4) 1/8,y,z

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2)
(2) 2 (0,0,1/2) 1/4,0,z
(3) d (3/4,0,3/4) x,1/8,z
(4) d (0,1/4,3/4) 3/8,y,z

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(2) 2 1/4,1/4,z
(3) d (3/4,0,1/4) x,3/8,z
(4) d (0,3/4,1/4) 3/8,y,z
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td>16 b 1 (1) x,y,z [u,v,w] (2) x+1/4,y+1/4,z+1/4 [u,v,w] (4) x+1/4,y+1/4,z+1/4 [u,v,w]</td>
</tr>
<tr>
<td>8 a .2 0,0,z [0,0,w] 1/4,1/4,z+1/4 [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg  
Along [1,0,0] c_p^-1m'1  
Along [0,1,0] c_p^-1m'1

a* = a/2  b* = b/2  
a* = b/2  b* = c/2  
a* = -a/2  b* = c/2

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
### Origin
on 112'

### Asymmetric unit

\[0 < x < \frac{1}{4};\quad 0 < y < \frac{1}{4};\quad 0 < z < 1\]

### Symmetry Operations

| For (0,0,0) + set |
|-------------------|---------------------------------|---------------------------------|
| (1) t (0,0,0)     | (2) 2 (0,0,0) z                 | (3) d (1/4,0,1/4) x, 1/8, z    |
|                   | (2z | 0,0,0)                      | (m, | 1/4,1/4,1/4)                  |
|                   |                                |                                | (m, | 1/4,1/4,1/4)                  |
|                   |                                |                                | For (0,1/2,1/2) + set          |
| (1) t (0,1/2,1/2) | (2) 2 (0,0,1/2) z               | (3) d (1/4,0,3/4) x, 3/8, z    |
|                   | (2z | 0,1/2,1/2)                    | (m, | 1/4,3/4,3/4)                  |
|                   |                                |                                | (m, | 1/4,3/4,3/4)                  |
|                   |                                |                                | For (1/2,0,1/2) + set          |
| (1) t (1/2,0,1/2) | (2) 2 (0,0,1/2) z               | (3) d (3/4,0,3/4) x, 1/8, z    |
|                   | (2z | 1/2,0,1/2)                    | (m, | 3/4,1/4,3/4)                  |
|                   |                                |                                | (m, | 3/4,1/4,3/4)                  |
|                   |                                |                                | For (1/2,1/2,0) + set          |
| (1) t (1/2,1/2,0) | (2) 2 (1/4,1,4, z              | (3) d (3/4,0,1/4) x, 3/8, z    |
|                   | (2z | 1/2,1/2,0)                    | (m, | 3/4,3/4,1/4)                  |
|                   |                                |                                | (m, | 3/4,3/4,1/4)                  |
|                   |                                |                                | For (0,0,0)' + set             |
| (1) t' (0,0,0)'   | (2) 2' (0,0,0) z               | (3) d' (1/4,0,1/4) x, 1/8, z   |
|                   | (2z | 0,0,0)'                      | (m, | 1/4,1/4,1/4)'                 |
|                   |                                |                                | (m, | 1/4,1/4,1/4)'                 |
|                   |                                |                                | For (0,1/2,1/2)' + set         |
| (1) t' (0,1/2,1/2) | (2) 2' (0,0,1/2) z            | (3) d' (1/4,0,3/4) x, 3/8, z   |
|                   | (2z | 0,1/2,1/2)'                   | (m, | 1/4,3/4,3/4)'                 |
|                   |                                |                                | (m, | 1/4,3/4,3/4)'                 |
Continued

43.2.321

Fdd21'

For (1/2,0,1/2)' + set

(1) t' (1/2,0,1/2)
(1) t' (1/2,0,1/2)'

(2) 2' 0,0,1/2 1/4,0,z
(2) 2' 1/2,0,1/2)

(3) d' (3/4,0,3/4) x,1/8,z
(3) d' (3/4,1/4,3/4)'

(4) d' (0,1/4,3/4) 3/8,y,z
(4) d' (3/4,1/4,3/4)'

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(1) t' (1/2,1/2,0)'

(2) 2' 1/4,1/4,z
(2) 2' 1/2,1/2,0')

(3) d' (3/4,0/1,4) x,3/8,z
(3) d' (3/4,3/4,1/4)'

(4) d' (0,3/4,1/4) 3/8,y,z
(4) d' (3/4,3/4,1/4)'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
(0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)' +

16 b 11' (1) x,y,z [0,0,0]  (2) x, y, z [0,0,0]  (3) x+1/4, y+1/4, z+1/4 [0,0,0]  (4) x+1/4, y+1/4, z+1/4 [0,0,0]

8 a ..21' 0,0,z [0,0,0]  1/4,1/4,z+1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2gg1'
Along [1,0,0] c1m11'
Along [0,1,0] c1m11'

\( a^* = a/2 \)  \( b^* = b/2 \)
\( a^* = b/2 \)  \( b^* = c/2 \)
\( a^* = -a/2 \)  \( b^* = c/2 \)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Fd'd2'  

Origin  on 112'

Asymmetric unit  
0 ≤ x ≤ 1/4;  
0 ≤ y ≤ 1/4;  
0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) t (0,0,0)  
(1 | 0,0,0)  
(2) 2' 0,0,z  
(2z | 0,0,0')  
(3) d (1/4,0,1/4) x,1/8,z  
(my | 1/4,1/4,1/4)  
(4) d' (0,1/4,1/4) 1/8,y,z  
(mx | 1/4,1/4,1/4')

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1 | 0,1/2,1/2)  
(2) 2' (0,0,1/2) 0,1/4,z  
(2z | 0,1/2,1/2')  
(3) d (1/4,0,3/4) x,3/8,z  
(my | 1/4,3/4,3/4)  
(4) d' (0,3/4,3/4) 1/8,y,z  
(mx | 1/4,3/4,3/4')

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2)  
(1 | 1/2,0,1/2)  
(2) 2' (0,0,1/2) 1/4,0,z  
(2z | 1/2,0,1/2')  
(3) d (3/4,0,3/4) x,1/8,z  
(my | 3/4,1/4,3/4)  
(4) d' (0,1/4,3/4) 3/8,y,z  
(mx | 3/4,1/4,3/4')

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1 | 1/2,1/2,0)  
(2) 2' 1/4,1/4,z  
(2z | 1/2,1/2,0')  
(3) d (3/4,0,1/4) x,3/8,z  
(my | 3/4,3/4,1/4)  
(4) d' (0,3/4,1/4) 3/8,y,z  
(mx | 3/4,3/4,1/4')
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
(0,0,0) + & (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + \\
16 & b \\ & 1 \\
&(1) x,y,z [u,v,w] \\
&(2) x+1/4,y,z+1/4 [u,v,w] \\
&(3) x+1/4,y+1/4,z+1/4 [u,v,w] \\
&(4) x,y+1/4,z+1/4 [u,v,w]
\end{align*}
\]

\[
\begin{align*}
8 & a \\ & .2' \\
&(0,0,z [u,v,0] \\
&1/4,1/4,z+1/4 [u,v,0]
\end{align*}
\]

Symmetry of Special Projections

Along [0,0,1] \( p2'gg' \) \quad Along [1,0,0] \( c1m1 \) \quad Along [0,1,0] \( c_{p}1m1 \)
\[
\begin{align*}
a^* &= -b/2 & b^* &= a/2 \\
a^* &= b/2 & b^* &= c/2 \\
a^* &= -a/2 & b^* &= c/2 \\
\text{Origin at 0,0,z} & & \text{Origin at x,0,0} & & \text{Origin at 0,y,0}
\end{align*}
\]
Fd'd'2 Orthorhombic

43.4.323

m'm'2

Fd'd'2

Origin on 112

Asymmetric unit

\[0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1\]

Symmetry Operations

For \((0,0,0)\) + set

\[
(1) \quad 1 \\
(2) \quad 2 \quad 0,0,z \\
(3) \quad d' \quad (1/4,0,1/4) \quad x,1/8,z \\
(4) \quad d' \quad (0,1/4,1/4) \quad 1/8,y,z
\]

\[
(1') \quad 0,0,0 \\
(2') \quad 0,0,0 \\
(3') \quad (m_y \cdot 1/4,1/4,1/4)' \\
(4') \quad (m_y \cdot 1/4,1/4,1/4)'
\]

For \((0,1/2,1/2)\) + set

\[
(1) \quad t (0,1/2,1/2) \\
(2) \quad 2 \quad 0,1/2,1/2 \quad 0,1/4,z \\
(3) \quad d' \quad (1/4,0,3/4) \quad x,3/8,z \\
(4) \quad d' \quad (0,3/4,3/4) \quad 1/8,y,z
\]

\[
(1') \quad 0,1/2,1/2 \\
(2') \quad 0,1/2,1/2 \\
(3') \quad (m_y \cdot 1/4,3/4,3/4)' \\
(4') \quad (m_y \cdot 1/4,3/4,3/4)'
\]

For \((1/2,0,1/2)\) + set

\[
(1) \quad t (1/2,0,1/2) \\
(2) \quad 2 \quad 0,1/2,0 \quad 1/4,0,z \\
(3) \quad d' \quad (3/4,0,3/4) \quad x,1/8,z \\
(4) \quad d' \quad (0,1/4,3/4) \quad 3/8,y,z
\]

\[
(1') \quad 1/2,0,1/2 \\
(2') \quad 1/2,0,1/2 \\
(3') \quad (m_y \cdot 3/4,1/4,3/4)' \\
(4') \quad (m_y \cdot 3/4,1/4,3/4)'
\]

For \((1/2,1/2,0)\) + set

\[
(1) \quad t (1/2,1/2,0) \\
(2) \quad 2 \quad 1/4,1/4,z \\
(3) \quad d' \quad (3/4,0,1/4) \quad x,3/8,z \\
(4) \quad d' \quad (0,3/4,1/4) \quad 3/8,y,z
\]

\[
(1') \quad 1/2,1/2,0 \\
(2') \quad 1/2,1/2,0 \\
(3') \quad (m_y \cdot 3/4,3/4,1/4)' \\
(4') \quad (m_y \cdot 3/4,3/4,1/4)'
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +

16 b 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x+1/4,y+1/4,z+1/4 [u,v,w] (4) x+1/4,y+1/4,z+1/4 [u,v,w]

8 a .2 0,0,z [0,0,w] 1/4,1/4,z+1/4 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p2g'g' Along [1,0,0] c1m'1 Along [0,1,0] c1m'1
a* = a/2  b* = b/2 a* = b/2  b* = c/2 a* = -a/2 b* = c/2
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
**Origin** on mm2

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

1. \(1\)  
2. \(2 \ 0,0,z\)  
3. \(m \ x,0,z\)  
4. \(m \ 0,y,z\)

\[
\begin{align*}
(1) & \ (1,0,0,0) \\
(2) & \ (2_z,0,0,0) \\
(3) & \ (m,0,0,0) \\
(4) & \ (m,0,0,0)
\end{align*}
\]

For \((1/2,1/2,1/2) + \text{ set}\)

1. \(t\) \((1/2,1/2,1/2)\)  
2. \(2 \ (0,0,1/2) \ 1/4,1/4,z\)  
3. \(n \ (1/2,0,1/2) \ x,1/4,z\)  
4. \(n \ (0,1/2,1/2) \ 1/4,y,z\)

\[
\begin{align*}
(1) & \ (1/2,1/2,1/2) \\
(2) & \ (2_z,1/2,1/2,1/2) \\
(3) & \ (m,1/2,1/2,1/2) \\
(4) & \ (m,1/2,1/2,1/2)
\end{align*}
\]
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicities,
Wyckoff letter,
Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

8 e 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]

4 d m.. 0,y,z [u,0,0] 0,y,z [u,0,0]

4 c .m. x,0,z [0,v,0] x,0,z [0,v,0]

2 b mm2 0,1/2,z [0,0,0]
2 a mm2 0,0,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm Along [1,0,0] c1m11' Along [0,1,0] c1m11'

a* = a  b* = b
Origin at 0,0,z

a* = b  b* = c
Origin at x,0,0

a* = -a  b* = c
Origin at 0,y,0
**Origin** on mm21'

**Asymmetric unit**  0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

1. 1
   (1) 1
   (2) 2  0,0,z
   (3) m  x,0,z
   (4) m  0,y,z
   (1*) 0,0,0
   (2*) 0,0,0
   (3*) m* 0,0,0
   (4*) m* 0,0,0

For (1/2,1/2,1/2) + set

1. t (1/2,1/2,1/2)
   (2) 2  0,0,1/2
   (3) n  1/2,0,1/2
   (4) n  1/2,1/2,1/2
   (1*) 1/2,1/2,1/2
   (2*) 1/2,1/2,1/2
   (3*) n* 1/2,1/2,1/2
   (4*) n* 1/2,1/2,1/2

For (0,0,0)' + set

1. 1'
   (1) 1'
   (2) 2' 0,0,z
   (3) m' x,0,z
   (4) m' 0,y,z
   (1*) 0,0,0'
   (2*) 0,0,0'
   (3*) m* 0,0,0'
   (4*) m* 0,0,0'

For (1/2,1/2,1/2)' + set

1. t' (1/2,1/2,1/2)
   (2) 2' 0,0,1/2
   (3) n' 1/2,0,1/2
   (4) n' 1/2,1/2,1/2
   (1*) 1/2,1/2,1/2'
   (2*) 1/2,1/2,1/2'
   (3*) n* 1/2,1/2,1/2'
   (4*) n* 1/2,1/2,1/2'
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)′ + (1/2,1/2,1/2)′ +</td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)′ + (1/2,1/2,1/2)′ +</td>
</tr>
<tr>
<td>8 e 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]</td>
<td>8 e 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 d m..1' 0,y,z [0,0,0] 0,y,z [0,0,0]</td>
<td>4 d m..1' 0,y,z [0,0,0] 0,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 c .m.1' x,0,z [0,0,0] x,0,z [0,0,0]</td>
<td>4 c .m.1' x,0,z [0,0,0] x,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 b mm21' 0,1/2,z [0,0,0]</td>
<td>2 b mm21' 0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 a mm21' 0,0,z [0,0,0]</td>
<td>2 a mm21' 0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] c2mm1'</th>
<th>Along [1,0,0] c1m11'</th>
<th>Along [0,1,0] c1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a′ = a  b′ = b</td>
<td>a′ = b  b′ = c</td>
<td>a′ = -a  b′ = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin on m'm2'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
   
   
   

2. $2', \quad 0,0,z$
   $\left(2', \quad 0,0,0\right)'$

3. $m, \quad x,0,z$
   $\left(m, \quad 0,0,0\right)'$

4. $m', \quad 0,y,z$
   $\left(m, \quad 0,0,0\right)'$

For $(1/2,1/2,1/2) +$ set

1. $t (1/2,1/2,1/2)$
   $\left(1/2,1/2,1/2\right)$

2. $2' (0,0,1/2) \quad 1/4,1/4,z$
   $\left(2, \quad 1/2,1/2,1/2\right)'$

3. $n (1/2,0,1/2) \quad x,1/4,z$
   $\left(m, \quad 1/2,1/2,1/2\right)'$

4. $n' (0,1/2,1/2) \quad 1/4,y,z$
   $\left(m, \quad 1/2,1/2,1/2\right)'$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 d m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 b m'm2'</td>
<td>0,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>2 a m'm2'</td>
<td>0,0,z [0,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( c2\)'mm'  \( a^* = -b \) \( b^* = a \)  \( a^* = -a \) \( b^* = c \)
Along [1,0,0] \( c1m1 \)  \( a^* = b \) \( b^* = c \)  \( a^* = b \) \( b^* = c \)
Along [0,1,0] \( c1m11' \)  \( a^* = b \) \( b^* = c \)  \( a^* = b \) \( b^* = c \)
Im'm'2 m'm'2 Orthorhombic

44.4.327

Origin on m'm'2

Asymmetric unit $0 < x < 1/2; \ 0 < y < 1/2; \ 0 < z < 1/2$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1
   (1 | 0,0,0)

(2) 2 0,0,z
(2z | 0,0,0)

(3) m' x,0,z
(mz | 0,0,0)'

(4) m' 0,y,z
(mz | 0,0,0)'

For $(1/2,1/2,1/2) +$ set

(1) t (1/2,1/2,1/2)
   (1 | 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2z | 1/2,1/2,1/2)

(3) n' (1/2,0,1/2) x,1/4,z
(mz | 1/2,1/2,1/2)'

(4) n' (0,1/2,1/2) 1/4,y,z
(mz | 1/2,1/2,1/2)'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>8  e  1  (1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4  d  m'.. 0,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>4  c  m'.. 0,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>2  b  m'.. 0,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>2  a  m'.. 0,y,z [0,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]  c2m'm'</th>
<th>Along [1,0,0]  c1m'1</th>
<th>Along [0,1,0]  c1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) ( b^* = b )</td>
<td>( a^* = b ) ( b^* = c )</td>
<td>( a^* = -a ) ( b^* = c )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin on mm2

Asymmetric unit

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For \((0,0,0) + \) set

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad m \quad x,0,z \\
(4) & \quad m \quad 0,y,z
\end{align*}

\begin{align*}
(1^* & \quad 0,0,0) \\
(2^* & \quad 0,0,0) \\
(3^* & \quad 0,0,0) \\
(4^* & \quad 0,0,0)
\end{align*}

For \((\frac{1}{2},\frac{1}{2},\frac{1}{2})' + \) set

\begin{align*}
(1) & \quad t' \quad (1/2,1/2,1/2) \\
(2) & \quad 2' \quad (0,0,1/2) \quad 1/4,1/4,z \\
(3) & \quad n' \quad (1/2,0,1/2) \quad x,1/4,z \\
(4) & \quad n' \quad (0,1/2,1/2) \quad 1/4,y,z
\end{align*}

\begin{align*}
(1^* & \quad 1/2,1/2,1/2) \\
(2^* & \quad 1/2,1/2,1/2) \\
(3^* & \quad 1/2,1/2,1/2) \\
(4^* & \quad 1/2,1/2,1/2)
\end{align*}
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
<tr>
<td>8 e 1 (1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 d m.. 0,y,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 c .m. x,0,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 b mm2 0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a mm2 0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c\textsubscript{p}-2mm

\(a^* = a\quad b^* = b\)

Origin at 0,0,z

Along [1,0,0] c1m11'

\(a^* = b\quad b^* = c\)

Origin at x,0,0

Along [0,1,0] c1m11'

\(a^* = -a\quad b^* = c\)

Origin at 0,y,0
Origin on mm'2'

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \]

Symmetry Operations

For (0,0,0) + set

1. \( \text{1} \)
   \( (1|0,0,0) \)

2. \( 2' \)
   \( 0,0,z \)
   \( (2|0,0,0)' \)

3. \( m' \)
   \( x,0,z \)
   \( (m|0,0,0)' \)

4. \( m \)
   \( 0,y,z \)
   \( (m|0,0,0) \)

For (1/2,1/2,1/2)' + set

1. \( t' \)
   \( (1|1/2,1/2,1/2) \)
   \( (1|1/2,1/2,1/2)' \)

2. \( 2 \)
   \( (0,0,1/2) \)
   \( 1/4,1/4,z \)
   \( (2|1/2,1/2,1/2) \)

3. \( n \)
   \( (1/2,0,1/2) \)
   \( x,1/4,z \)
   \( (m|1/2,1/2,1/2) \)

4. \( n' \)
   \( (0,1/2,1/2) \)
   \( 1/4,y,z \)
   \( (m|1/2,1/2,1/2)' \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>8 e 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 d m.. 0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 c m'. x,0,z [u,0,w]</td>
<td>x,0,z [u,0,\bar{w}]</td>
</tr>
<tr>
<td>2 b mm'2' 0,1/2,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a mm'2' 0,0,z [u,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c_p 2'mm'</th>
<th>Along [1,0,0] c1m11'</th>
<th>Along [0,1,0] c_p 1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = -a b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
**Origin** on \( m'm'2 \)

**Asymmetric unit**

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

1. \(1 \quad (0,0,0)\)
2. \(2 \quad 0,0,z \quad (1/2,0,0,0)\)
3. \(m' \quad x,0,z\quad (m_x,0,0)\)
4. \(m' \quad 0,y,z\quad (m_x,0,0)\)

For \((1/2,1/2,1/2)' + \text{ set}\)

1. \(t' \quad (1/2,1/2,1/2)\)
2. \(2' \quad 0,0,1/2 \quad 1/4,1/4,z\)
3. \(n \quad (1/2,0,1/2) \quad x,1/4,z\)
4. \(n \quad (0,1/2,1/2) \quad 1/4,y,z\)

\[ \text{44.7.330 - 1 - 636} \]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>f e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>f d m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>f c m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>g b m'm'2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>g a m'm'2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_p.2m'm'  
Along [1,0,0] c_p.1m'1  
Along [0,1,0] c_p.1m'1

a* = a  b* = b  
a* = b  b* = c  
a* = -a  b* = c

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin on cc2

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0) + \text{ set}\)

1. \((1)\) 1
   \(1)\) 0,0,0
2. \((2)\) 0,0,z
   \(2)\) 0,0,0
3. \((3)\) c (0,0,1/2) x,0,z
   \(3)\) c (0,0,1/2) 0,0,0
4. \((4)\) c (0,0,1/2) 0,y,z
   \(4)\) c (0,0,1/2) 0,0,0

For \((1/2,1/2,1/2) + \text{ set}\)

1. \((1)\) t (1/2,1/2,1/2)
   \(1)\) t (1/2,1/2,1/2)
2. \((2)\) 2 (0,0,1/2) 1/4,1/4,z
   \(2)\) 2 (0,0,1/2) 1/2,1/2,1/2
3. \((3)\) a (1/2,0,0) x,1/4,z
   \(3)\) a (1/2,0,0) 1/2,1/2,0
4. \((4)\) b (0,1/2,0) 1/4,y,z
   \(4)\) b (0,1/2,0) 1/2,1/2,0
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>8 c 1 (1) x,y,z [u,v,w]</th>
<th>4 b ..2 0,1/2,z [0,0,w]</th>
<th>4 a ..2 0,0,z [0,0,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm
\[ \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] \( p_{2a} \cdot 1 m'1 \)
\[ \mathbf{a}^* = \mathbf{b}/2, \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x,0,0

Along [0,1,0] \( p_{2b} \cdot 1 m'1 \)
\[ \mathbf{a}^* = -\mathbf{a}/2, \mathbf{b}^* = \mathbf{c}/2 \]
Origin at 0,y,0
Origin on cc21'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) t (1/2,1/2,1/2)
(1) t' (1/2,1/2,1/2)

(2) 2 0,0,z
(2) 2 (0,0,1/2) 1/4,1/4,z
(2) 2' (0,0,1/2) 1/4,1/4,z

(3) c (0,0,1/2) x,0,z
(3) a (1/2,0,0) x,1/4,z
(3) c' (0,0,1/2) x,0,z
(3) a' (1/2,0,0) x,1/4,z

(4) c (0,0,1/2) 0,y,z
(4) b (0,1/2,0) 1/4,y,z
(4) c' (0,0,1/2) 0,y,z
(4) b' (0,1/2,0) 1/4,y,z

For (1/2,1/2,1/2) + set

(1) 1
(1) t (1/2,1/2,1/2)
(1) t' (1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2) 2 (0,0,1/2) 1/4,1/4,z

(3) a (1/2,0,0) x,1/4,z
(3) a' (1/2,0,0) x,1/4,z

(4) b (0,1/2,0) 1/4,y,z
(4) b' (0,1/2,0) 1/4,y,z

For (0,0,0)′ + set

(1) 1′
(1) t' (1/2,1/2,1/2)
(1) t′ (1/2,1/2,1/2)

(2) 2′ 0,0,z
(2) 2′ (0,0,1/2) 1/4,1/4,z

(3) c′ (0,0,1/2) x,0,z
(3) a (1/2,0,0) x,1/4,z

(4) c′ (0,0,1/2) 0,y,z
(4) b (0,1/2,0) 1/4,y,z

For (1/2,1/2,1/2)′ + set

(1) 1′
(1) t′ (1/2,1/2,1/2)
(1) t′ (1/2,1/2,1/2)

(2) 2′ (0,0,1/2) 1/4,1/4,z
(2) 2′ (0,0,1/2) 1/4,1/4,z

(3) a′ (1/2,0,0) x,1/4,z
(3) a' (1/2,0,0) x,1/4,z

(4) b′ (0,1/2,0) 1/4,y,z
(4) b' (0,1/2,0) 1/4,y,z
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 11'</td>
<td>(1) x,y,z [0,0,0] (2) x,$\bar{y}$,z+1/2 [0,0,0] (3) x,$\bar{y}$,z+1/2 [0,0,0] (4) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b ..21'</td>
<td>0,1/2,z [0,0,0] 0,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a ..21'</td>
<td>0,0,z [0,0,0] 0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along $[0,0,1]$ c2mm1'  Along $[1,0,0]$ p1m11'  Along $[0,1,0]$ p1m11'

$\mathbf{a}^* = \mathbf{a}$  $\mathbf{b}^* = \mathbf{b}$  $\mathbf{a}^* = \mathbf{b}/2$  $\mathbf{b}^* = \mathbf{c}/2$  $\mathbf{a}^* = -\mathbf{a}/2$  $\mathbf{b}^* = \mathbf{c}/2$

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Ib'a2'  m'm2'  Orthorhombic
45.3.333  Ib'a2'

Origin  on c'c2'

Asymmetric unit  0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2' 0,0,z
(3) c (0,0,1/2) x,0,z
(4) c' (0,0,1/2) 0,y,z

(1*) 0,0,0
(2*) 0,0,0'
(3*) (0,0,1/2) (m,0,0,1/2)
(4*) (0,0,1/2') (m,0,0,1/2')

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(2) 2' (0,0,1/2) 1/4,1/4,z
(3) a (1/2,0,0) x,1/4,z
(4) b' (0,1/2,0) 1/4,y,z

(1*) 1/2,1/2,1/2
(2*) 1/2,1/2,1/2'
(3*) (1/2,0,0) (m,1/2,1/2,0)
(4*) (0,1/2,0) (m,1/2,1/2,0)'

45.3.333 - 1 - 642
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
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<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>8  c  1  (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4  b  .2'  0,1/2,z [u,v,0]</td>
<td>0,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4  a  .2'  0,0,z [u,v,0]</td>
<td>0,0,z+1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] c2'mm'  
  \( \mathbf{a^*} = -\mathbf{b} \quad \mathbf{b^*} = \mathbf{a} \)  
  Origin at 0,0,z

- Along [1,0,0] p1m1  
  \( \mathbf{a^*} = \mathbf{b} / 2 \quad \mathbf{b^*} = \mathbf{c} / 2 \)  
  Origin at x,0,0

- Along [0,1,0] p̄21m1  
  \( \mathbf{a^*} = -\mathbf{a} / 2 \quad \mathbf{b^*} = \mathbf{c} / 2 \)  
  Origin at 0,y,0
Origin on c'c'2

Asymmetric unit  
\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2} \]

Symmetry Operations

For \((0,0,0) + \) set

1. \((1,0,0,0)\)
2. \(0,0,z\)
3. \(c'(0,0,1/2), x,0,z\)  
4. \(c'(0,0,1/2), 0,y,z\)

For \((1/2,1/2,1/2) + \) set

1. \(t(1/2,1/2,1/2)\)
2. \((0,0,1/2), 1/4,1/4,z\)  
3. \(a'(1/2,0,0), x,1/4,z\)  
4. \(b'(0,1/2,0), 1/4,y,z\)

\[ 45.4.334 \quad \text{lb'a'2} \quad \text{Orthorhombic} \]
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**  

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<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b 2</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 a 2</td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 a 2</td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**  

<table>
<thead>
<tr>
<th>Along [0,0,1] c2m'</th>
<th>Along [1,0,0] p1m'1</th>
<th>Along [0,1,0] p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) ( b^* = b )</td>
<td>( a^* = b/2 ) ( b^* = c/2 )</td>
<td>( a^* = -a/2 ) ( b^* = c/2 )</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
**Origin**  on cc2

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

- $(1) \ 1$
- $(2) \ 2 \quad 0,0,z$
- $(3) \ c \quad (0,0,1/2) \quad x,0,z$
- $(4) \ c \quad (0,0,1/2) \quad 0,y,z$

For (1/2,1/2,1/2)' + set

- $(1) \ t' \quad (1/2,1/2,1/2)'$
- $(2) \ 2' \quad (0,0,1/2) \quad 1/4,1/4,z$
- $(3) \ a' \quad (1/2,0,0) \quad x,1/4,z$
- $(4) \ b' \quad (0,1/2,0) \quad 1/4,y,z$

$(m, 0,0,1/2)$

$(m, 1/2,1/2,0)'$

$(m, 1/2,1/2,0)'$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 b .2</td>
<td>0,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Coordinates

(0,0,0) + (1/2,1/2,1/2)' +

(2) x,y,z [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x,y,z+1/2 [u,v,w]

Symmetry of Special Projections

Along [0,0,1] c_p,2mm
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p_2b,1m'1
a* = b/2  b* = c/2
Origin at x,0,0

Along [0,1,0] p_2b,1m'1
a* = -a/2 b* = c/2
Origin at 0,y,0
I\textsubscript{h}ba'2'  
mm21'  
Orthorhombic  
45.6.336  
I\textsubscript{h}ba'2'

**Origin** on cc'2'

**Asymmetric unit**

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2} \]

**Symmetry Operations**

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2' \quad 0,0,z \\
(3) & \quad c' \quad (0,0,1/2) \quad x,0,z \\
(4) & \quad c \quad (0,0,1/2) \quad 0,y,z \\
(1^* & \quad 0,0,0) \\
(2^* & \quad 0,0,0)' \\
(3^* & \quad 0,0,1/2)' \\
(4^* & \quad 0,0,1/2)'
\end{align*}
\]

For \((1/2,1/2,1/2)' + \) set

\[
\begin{align*}
(1) & \quad t' \quad (1/2,1/2,1/2) \\
(2) & \quad 2 \quad (0,0,1/2) \quad 1/4,1/4,z \\
(3) & \quad a \quad (1/2,0,0) \quad x,1/4,z \\
(4) & \quad b' \quad (0,1/2,0) \quad 1/4,y,z \\
(1^* & \quad 1/2,1/2,1/2) \\
(2^* & \quad 1/2,1/2,1/2) \\
(3^* & \quad 1/2,0,0) \\
(4^* & \quad 1/2,1/2,0)'
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
<td></td>
</tr>
</tbody>
</table>

8 c 1  (1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) x,y,z+1/2 [u,v,w]  (4) x,y,z+1/2 [u,v,w]
4 b ..2'  0,1/2,z [u,v,0]  0,1/2,z+1/2 [u,v,0]
4 a ..2'  0,0,z [u,v,0]  0,0,z+1/2 [u,v,0]

Symmetry of Special Projections

Along [0,0,1] c_p,2'mm'  Along [1,0,0] p_{2a}.1m1  Along [0,1,0] p_{2a}.1m1
\textbf{a}^{*} = \textbf{a}  \quad \textbf{b}^{*} = \mathbf{b}  \quad \textbf{a}^{*} = \mathbf{b}/2  \quad \textbf{b}^{*} = \mathbf{c}/2  \quad \textbf{a}^{*} = -\mathbf{a}/2  \quad \textbf{b}^{*} = \mathbf{c}/2
Origin at 0,0,z  \quad \text{Origin at } x,0,0  \quad \text{Origin at } 0,y,0
Origin on c’c’2

Asymmetric unit  
0 < x < 1/2;  
0 < y < 1/2;  
0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1 | 0,0,0)

(2) 2 0,0,z
    (2 | 0,0,0)

(3) c’ (0,0,1/2) x,0,z
    (m | 0,0,1/2)’

(4) c’ (0,0,1/2) 0,y,z
    (m | 0,0,1/2)’

For (1/2,1/2,1/2)’ + set

(1) t’ (1/2,1/2,1/2)’
    (1 | 1/2,1/2,1/2)’

(2) 2’ (0,0,1/2) 1/4,1/4,z
    (2 | 1/2,1/2,1/2)’

(3) a (1/2,0,0) x,1/4,z
    (m | 1/2,1/2,0)

(4) b (0,1/2,0) 1/4,y,z
    (m | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

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</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] \( c_{a}^{p}2m'm' \)  
  \( a^* = a \)  \( b^* = b \)  
  Origin at 0,0,z

- Along [1,0,0] \( p_{2b}1m1 \)  
  \( a^* = b/2 \)  \( b^* = c/2 \)  
  Origin at x,0,0

- Along [0,1,0] \( p_{2a}1m1 \)  
  \( a^* = -a/2 \)  \( b^* = c/2 \)  
  Origin at 1/4,y,0
**Origin** on na2

**Asymmetric unit**

\[ 0 < x < \frac{1}{4}; \quad 0 < y < 1; \quad 0 < z < \frac{1}{2} \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(T\)
2. \(2 \ 0,0,z\)
3. \(a \ (1/2,0,0) \ x,0,z\)
4. \(m \ 1/4,y,z\)

\(n_{0,0,0}\)
\(n_{1/2,0,0}\)
\(n_{0,1/2,0}\)
\(n_{1/2,1/2,0}\)

For \((1/2,1/2,1/2)\) + set

1. \(t \ (1/2,1/2,1/2)\)
2. \(2 \ (0,1/2) \ 1/4,1/4,z\)
3. \(c \ (0,0,1/2) \ x,1/4,z\)
4. \(n \ (0,1/2,1/2) \ 0,y,z\)

\(n_{1/2,1/2,1/2}\)
\(n_{1/2,1/2,1/2}\)
\(n_{0,1/2,1/2}\)
\(n_{0,1/2,1/2}\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Site Symmetry</th>
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<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>4 b m..</td>
<td>1/4,y,z [u,0,0]</td>
<td>3/4,y,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
<td></td>
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</table>

Symmetry of Special Projections

Along [0,0,1] c2mm  Along [1,0,0] c1m11'  Along [0,1,0] p2 règle 1m1

a* = a  b* = b  a* = b  b* = c  a* = -a/2  b* = c/2

Origin at 1/4,1/4,z  Origin at x,0,0  Origin at 0,y,0
Origin on na21'

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. 1
   (1) (0,0,0)
   (2) (0,0,z)
   (3) a (1/2,0,0) x,0,z
   (4) m 1/4,y,z

For (1/2,1/2,1/2) + set

1. t (1/2,1/2,1/2)
   (1) (1/2,1/2,1/2)
   (2) (0,0,1/2) 1/4,1/4,z
   (3) c (0,0,1/2) x,1/4,z
   (4) n (0,1/2,1/2) 0,y,z

For (0,0,0)' + set

1. t' (1/2,1/2,1/2)
   (1) (1/2,1/2,1/2)
   (2) (0,0,1/2) 1/4,1/4,z
   (3) a' (1/2,0,0) x,0,z
   (4) m' 1/4,y,z

For (1/2,1/2,1/2)' + set

1. t' (1/2,1/2,1/2)
   (1) (1/2,1/2,1/2)
   (2) (0,0,1/2) 1/4,1/4,z
   (3) c' (0,0,1/2) x,1/4,z
   (4) n' (0,1/2,1/2) 0,y,z

46.1.338 - 3 - 654
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

Positions

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<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
</tbody>
</table>

8 c 11' (1) x,y,z [0,0,0] (2) x,y,3/2 [0,0,0] (3) x+1/2,y,1/2 [0,0,0] (4) x+1/2,y,3/2 [0,0,0]

4 b m..1' 1/4,y,z [0,0,0] 3/4,y,1/2 [0,0,0]

4 a ..21' 0,0,z [0,0,0] 1/2,0,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,0,0] c1m11' Along [0,1,0] p1m11'

a* = a  b* = b  a* = -a/2  b* = c/2

Origin at 1/4,1/4,0  Origin at x,0,0  Origin at 0,y,0
Origin on n'a2'

Asymmetric unit \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\)  
2. \(2'\) 0,0,z  
3. \(a\) (1/2,0,0) 0,x,z  
4. \(m'\) 1/4,y,z

For \((1/2,1/2,1/2) + \) set

1. \(t\) (1/2,1/2,1/2)  
2. \(2'\) (0,0,1/2) 1/4,1/4,z  
3. \(c\) (0,0,1/2) 0,1/4,z  
4. \(n'\) (0,1/2,1/2) 0,y,z

\[46.3.340 - 1 - 656\]
Generators selected  (1); t(1,0,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b m'..</td>
<td>1/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2mm'  Along [1,0,0]  c1m1  Along [0,1,0]  p2a,1m1
a* = -b  b* = a  a* = b  b* = c  a* = -a/2  b* = c/2
Origin at 1/4,1/4,z  Origin at x,0,0  Origin at 0,y,0
Origin  on na'2'

Asymmetric unit  0 ≤ x ≤ 1/4;  0 ≤ y ≤ 1;  0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1|0,0,0)
(2) 2'  0,0,z
   (2|0,0,0)'
(3) a' (1/2,0,0)  x,0,z
   (m,|1/2,0,0)'
(4) m  1/4,y,z
   (m,|1/2,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
   (1|1/2,1/2,1/2)
(2) 2'  (0,0,1/2)  1/4,1/4,z
   (2|1/2,1/2,1/2)'
(3) c' (0,0,1/2)  x,1/4,z
   (m,|0,1/2,1/2)'
(4) n (0,1/2,1/2)  0,y,z
   (m,|0,1/2,1/2)
Generators selected  
(1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>4</td>
<td>b m</td>
<td>1/4,y,z [u,0,0]</td>
<td>3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>a .2'</td>
<td>0,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2"mm'  Along [1,0,0] c1"m1'  Along [0,1,0] p1m1
\( a^* = a \quad b^* = b \)  \( a^* = b \quad b^* = c \)  \( a^* = -\frac{a}{2} \quad b^* = \frac{c}{2} \)
Origin at 1/4,1/4,z  Origin at x,0,0  Origin at 0,y,0
Im'a'2 m'm'2 Orthorhombic
46.5.342 Im'a'2

**Origin** on n'a'2

**Asymmetric unit**

\[ 0 < x < \frac{1}{4}; \quad 0 < y < 1; \quad 0 < z < \frac{1}{2} \]

**Symmetry Operations**

For \((0,0,0)\) + set:

1. \(1\)
2. \(2 \quad 0,0,z\)
3. \(a' (1/2,0,0) \quad x,0,z\)
4. \(m' (1/4,y,z)\)

For \((1/2,1/2,1/2)\) + set:

1. \(t (1/2,1/2,1/2)\)
2. \(2 (0,0,1/2) \quad 1/4,1/4,z\)
3. \(c' (0,0,1/2) \quad x,1/4,z\)
4. \(n' (0,1/2,1/2) \quad 0,y,z\)

\((1) 0,0,0\) \quad \((2) z\) \quad \((3) y\) \quad \((4) x\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 b m'..</td>
<td>1/4,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3/4,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2m'm'  
\( a^* = a \) \( b^* = b \)  
Origin at 1/4,1/4,z

Along [1,0,0] c1m'1  
\( a^* = b \) \( b^* = c \)  
Origin at x,0,0

Along [0,1,0] p1m'1  
\( a^* = -a/2 \) \( b^* = c/2 \)  
Origin at 0,y,0
Origin on n'a2

Asymmetric unit $0 \leq x \leq 1/4$; $0 \leq y \leq 1$; $0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) + \text{ set}$

(1) $1$

(2) $2$ 0,0,z

(3) a $(1/2,0,0)$ x,0,z

(4) m 1/4,y,z

For $(1/2,1/2,1/2)' + \text{ set}$

(1) t' $(1/2,1/2,1/2)$

(2) $2'$ $(0,0,1/2)$ 1/4,1/4,z

(3) c' $(0,0,1/2)$ x,1/4,z

(4) n' $(0,1/2,1/2)$ 0,y,z
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x, y, z [u, v, w]</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>4 b m..</td>
<td>1/4, y, z [u, 0, 0]</td>
<td>3/4, y, z [u, 0, 0]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0, 0, z [0, 0, w]</td>
<td>1/2, 0, z [0, 0, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_p, 2'nm'  
Along [1,0,0] c1m11'  
Along [0,1,0] p_{2a}.1m1  

a* = a  b* = b  
Origin at 1/4, 1/4, z  

a* = b  b* = c  
Origin at x, 0, 0  

a* = -a/2  b* = c/2  
Origin at 1/4, y, 0
Origin  on na’2

Asymmetric unit  0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2’ 0,0,z
(3) a (1/2,0,0) x,0,z
(4) m’ 1/4,y,z
(m_y | 1/2,0,0)

For (1/2,1/2,1/2)’ + set

(1) t’ (1/2,1/2,1/2)
(2) 2 (0,0,1/2) 1/4,1/4,z
(3) c’ (0,0,1/2) x,1/4,z
(4) n (0,1/2,1/2) 0,y,z
(m_x | 0,1/2,1/2)

46.7.344 - 1 - 664
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>(1/2,1/2,1/2) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b m'</td>
<td>1/4,x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_p 2m'm'  
Along [1,0,0] c_p'1m1  
Along [0,1,0] p_2a1m1

a* = a b* = b  
a* = b b* = c  
a* = -a/2 b* = c/2

Origin at 1/4,1/4,z  
Origin at x,0,0  
Origin at 0,y,0
Origin on n'a'2'

Asymmetric unit \(0 \leq x \leq 1/4\); \(0 \leq y \leq 1\); \(0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\)
2. \(2'\) \(0,0,z\)
3. \(a'(1/2,0,0)\) \(x,0,z\)
4. \(m\) \(1/4,y,z\)

For \((1/2,1/2,1/2)' + \) set

1. \(t'(1/2,1/2,1/2)\)
2. \(2\) \(0,0,1/2\) \(1/4,1/4,z\)
3. \(c\) \((0,0,1/2)\) \(x,1/4,z\)
4. \(n'(0,1/2,1/2)\) \(0,y,z\)
Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>SiteSymmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b m..</td>
<td>1/4,y,z [u,0,0]</td>
<td>(2)</td>
<td>3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>0,0,z [u,v,0]</td>
<td>(3)</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] cₚ,2mm
Along [1,0,0] c₁m11'
Along [0,1,0] p₂ᵥ,1m1

a$^*$ = a b$^*$ = b
a$^*$ = b b$^*$ = c
a$^*$ = -a/2 b$^*$ = c/2

Origin at 1/4,1/4,z
Origin at x,0,0
Origin at 0,y,0
Iₚm'a'2

mm21'

Origin on na'2

Asymmetric unit

\begin{align*}
0 \leq x & \leq 1/4; \\
0 \leq y & \leq 1; \\
0 \leq z & \leq 1/2
\end{align*}

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)
(2) 2' 0,0,z
(2|0,0,0)
(3) a' (1/2,0,0) x,0,z
(mₐ|1/2,0,0)'
(4) m' 1/4,y,z
(mₐ|1/2,0,0)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)
(1|1/2,1/2,1/2)'
(2) 2' (0,0,1/2) 1/4,1/4,z
(2|1/2,1/2,1/2)'
(3) c (0,0,1/2) x,1/4,z
(mₐ|1/2,1/2)
(4) n (0,1/2,1/2) 0,y,z
(mₐ|0,1/2,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b m'..</td>
<td>1/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 a ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c_p 2'mm'  
\( \mathbf{a}^* = \mathbf{-b}/2 \quad \mathbf{b}^* = \mathbf{a}/2 \)
Origin at 1/4,1/4,z

Along [1,0,0]  c_p 1m'1  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)
Origin at x,0,0

Along [0,1,0]  p_{21} 1m'1  
\( \mathbf{a}^* = -\mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)
Origin at 0,y,0
**Orthorhombic**

Pmmm

47.1.347

Ormm

P2/m2/m2/m

**Origin** at center (mmm)

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

1. \(1\)
   
2. \(2 \ 0,0,z\)
   
3. \(2 \ 0,y,0\)
   
4. \(2 \ x,0,0\)

5. \(1\)

6. \(m \ x,y,0\)

7. \(m \ x,0,z\)

8. \(m \ 0,y,z\)

9. \(m \ 0,0,0\)
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8 α 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 z .m</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 y .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>4 x .m</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>4 w .m</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 v m..</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 u m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>2 t mm2</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 s mm2</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 r mm2</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 q mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 p m2m</td>
<td>1/2,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 o m2m</td>
<td>1/2,y,0 [0,0,0]</td>
</tr>
<tr>
<td>2 n m2m</td>
<td>0,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 m m2m</td>
<td>0,y,0 [0,0,0]</td>
</tr>
<tr>
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<td>x,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 k 2mm</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 j 2mm</td>
<td>x,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 i 2mm</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>1 h mmm</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 g mmm</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 f mmm</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1 e mmm</td>
<td>0,1/2,0 [0,0,0]</td>
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Continued

1 d mmm 1/2,0,1/2 [0,0,0]
1 c mmm 0,0,1/2 [0,0,0]
1 b mmm 1/2,0,0 [0,0,0]
1 a mmm 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2mm1’
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2mm1’
\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,0,0

Along [0,1,0] p2mm1’
\[ \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a} \]
Origin at 0,y,0
Origin at center (mmm1')

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For 1 + set:

1. $1 \quad [0,0,0]$
2. $2 \quad 0,0,z \quad [0,0,0]$
3. $2 \quad 0,y,0 \quad [0,0,0]$
4. $2 \quad x,0,0 \quad [0,0,0]$

For 1' + set:

1. $1' \quad [0,0,0]'$
2. $2' \quad 0,0,z \quad [0,0,0]'$
3. $2' \quad 0,y,0 \quad [0,0,0]'$
4. $2' \quad x,0,0 \quad [0,0,0]'$

5. $m \quad x,y,0 \quad [0,0,0]$
6. $m \quad x,0,z \quad [0,0,0]$
7. $m \quad x,0,z \quad [0,0,0]$
8. $m \quad 0,y,0 \quad [0,0,0]$

5. $m' \quad x,y,0 \quad [0,0,0]'$
6. $m' \quad x,0,z \quad [0,0,0]'$
7. $m' \quad x,0,z \quad [0,0,0]'$
8. $m' \quad 0,y,0 \quad [0,0,0]'$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>1 + 1' +</td>
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<tr>
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<td>1 g mmm1' 0,1/2,1/2 [0,0,0]</td>
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<td>1 e mmm1' 0,1/2,0 [0,0,0]</td>
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Continued

1. d. mmm1' 1/2,0,1/2 [0,0,0]
1. c. mmm1' 0,0,1/2 [0,0,0]
1. b. mmm1' 1/2,0,0 [0,0,0]
1. a. mmm1' 0,0,0 [0,0,0]

**Symmetry of Special Projections**

<table>
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<tr>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
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<tr>
<td>p2mm1'</td>
<td>p2mm1'</td>
<td>p2mm1'</td>
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<tr>
<td>( a^* = a )</td>
<td>( a^* = b )</td>
<td>( a^* = c )</td>
</tr>
<tr>
<td>( b^* = b )</td>
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<td>( b^* = a )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin \(\text{at center (m'\text{mm})}\)

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

\[
\begin{align*}
(1) \quad & 1 \\
(1) & (0,0,0) \\
(5) \quad & 1' \\
(1) & (0,0,0)' \\
(2) \quad & 2' \\
(2) & (0,0,z) \\
(2) & (0,0,0)' \\
(2) & (0,y,0) \\
(2) & (0,0,0)' \\
(3) \quad & 2' \\
(3) & (0,y,0) \\
(3) & (0,0,0)' \\
(4) \quad & 2 \\
(4) & (x,0,0) \\
(4) & (2_x,0,0) \\
(6) \quad & m \\
(6) & (x,y,0) \\
(6) & (m_z,0,0,0) \\
(7) \quad & m \\
(7) & (x,0,z) \\
(7) & (m_y,0,0,0) \\
(8) \quad & m' \\
(8) & (0,y,z) \\
(8) & (m_z,0,0,0)' \\
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<tbody>
<tr>
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<td>(1) x,y,z [u,v,w]</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] p2mm1’
\( a^* = a \) \( b^* = b \)
Origin at 0,0,z

Along [1,0,0] p2mm
\( a^* = b \) \( b^* = c \)
Origin at x,0,0

Along [0,1,0] p2mm1’
\( a^* = c \) \( b^* = a \)
Origin at 0,y,0
Origin at center (m'm'm)

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

(1) 1  \hspace{1cm} (2) 2  0,0,z  \hspace{1cm} (3) 2'  0,y,0  \hspace{1cm} (4) 2'  x,0,0  \\
    (1|0,0,0) \hspace{1cm} (2_z|0,0,0) \hspace{1cm} (2_y|0,0,0)' \hspace{1cm} (2_x|0,0,0)'

(5) 1'  \hspace{1cm} (6) m  x,y,0  \hspace{1cm} (7) m'  x,0,z  \hspace{1cm} (8) m'  0,y,z  \\
     (1'|0,0,0) \hspace{1cm} (m_z|0,0,0) \hspace{1cm} (m_y|0,0,0)' \hspace{1cm} (m_x|0,0,0)'

Orthorhombic

Pm'm'm

m'm'm

47.4.350

P2'/m'2'/m'2'/m
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>x,y,1/2 [0,0,w]</td>
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</tr>
<tr>
<td>2 m m'2'm</td>
<td>0,y,0 [0,0,w]</td>
<td>0,y,0 [0,0,w]</td>
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<td>x,0,0 [0,0,w]</td>
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<td>1/2,1/2,1/2 [0,0,w]</td>
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<td>1 e m'm'm</td>
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</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2m'm'</th>
<th>Along [1,0,0] p2'mm'</th>
<th>Along [0,1,0] p2'mm'</th>
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<tbody>
<tr>
<td>$\mathbf{a}^* = \mathbf{a}$</td>
<td>$\mathbf{b}^* = \mathbf{b}$</td>
<td>$\mathbf{a}^* = \mathbf{c}$</td>
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<tr>
<td>Origin at 0,0,z</td>
<td>Origin at 1,0,0</td>
<td>Origin at 0,1,0</td>
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</table>

<table>
<thead>
<tr>
<th>Along [0,0,1] p2m'm'</th>
<th>Along [1,0,0] p2'mm'</th>
<th>Along [0,1,0] p2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbf{a}^* = \mathbf{a}$</td>
<td>$\mathbf{b}^* = \mathbf{b}$</td>
<td>$\mathbf{a}^* = \mathbf{a}$</td>
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<tr>
<td>Origin at 0,0,z</td>
<td>Origin at 1,0,0</td>
<td>Origin at 0,1,0</td>
</tr>
</tbody>
</table>
**Origin** at center (m'm'm')

**Asymmetric unit** $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

1. $\begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix}$
2. $\begin{pmatrix} 2 \\ 0,0,z \end{pmatrix}$
3. $\begin{pmatrix} 2 \\ 0,y,0 \end{pmatrix}$
4. $\begin{pmatrix} 2 \\ x,0,0 \end{pmatrix}$
5. $\begin{pmatrix} 1' \\ 0,0,0' \end{pmatrix}$
6. $\begin{pmatrix} m' \\ x,y,0 \end{pmatrix}$
7. $\begin{pmatrix} m' \\ x,0,z \end{pmatrix}$
8. $\begin{pmatrix} m' \\ 0,y,z \end{pmatrix}$

**Orthorhombic**

- **Pm'm'm'**
  - 47.5.351

- **m'm'm'**
  - P2/m'2/m'/2/m'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<th>Multiplicity</th>
<th>Coordinates</th>
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<td>(3) $x,y,z [u,v,w]$</td>
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<td>(4) $x,y,z [u,v,w]$</td>
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<td>$x,0,0 [u,0,0]$</td>
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<tr>
<td>1 h m'</td>
<td>$1/2,1/2,1/2 [0,0,0]$</td>
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<tr>
<td>1 g m'</td>
<td>$0,1/2,1/2 [0,0,0]$</td>
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<td>1 f m'</td>
<td>$1/2,1/2,0 [0,0,0]$</td>
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<td>$0,1/2,0 [0,0,0]$</td>
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Continued

1  d  m'm'm'  1/2,0,1/2 [0,0,0]
1  c  m'm'm'  0,0,1/2 [0,0,0]
1  b  m'm'm'  1/2,0,0 [0,0,0]
1  a  m'm'm'  0,0,0 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2m'm'</th>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
<th>Along [0,1,0]</th>
<th>p2m'm'</th>
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<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = c</td>
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<td>Origin at x,0,0</td>
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<td>Origin at 0,y,0</td>
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</tbody>
</table>
**Symmetry Operations**

**For (0,0,0) + set**

1. $T (0,0,0)$
   - $(1) T (0,0,0)$
   - $(2) 2 0,0,z$  
     - $(2_x 0,0,0)$
   - $(3) 2 0,y,0$  
     - $(2_y 0,0,0)$
   - $(4) 2 x,0,0$  
     - $(2_z 0,0,0)$

2. $T (0,0,0)'$
   - $(5) T (0,0,0)'$
   - $(6) m x,y,0$  
     - $(m_x 0,0,0)$
   - $(7) m x,0,z$  
     - $(m_y 0,0,0)$
   - $(8) m 0,y,z$  
     - $(m_z 0,0,0)$

**For (1,0,0)' + set**

1. $T' (1,0,0)$
   - $(1) T' (1,0,0)$
   - $(2) 2' 1/2,0,z$  
     - $(2_x 1/2,0,0)'$
   - $(3) 2' 1/2,y,0$  
     - $(2_y 1/2,0,0)'$
   - $(4) 2' (1,0,0) x,0,0$  
     - $(2_z 1/2,0,0)'$

2. $T' (1/2,0,0)$
   - $(5) T' (1/2,0,0)$
   - $(6) a' (1,0,0) x,y,0$  
     - $(a'_x 1,0,0)'$
   - $(7) a' (1,0,0) x,0,z$  
     - $(a'_y 1,0,0)'$
   - $(8) m' 1/2,y,z$  
     - $(m'_z 1,0,0)'$

**Origin** at center (mmm)

**Asymmetric unit**  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2
Generators selected  (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity,
Wyckoff letter,
Site Symmetry.

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<td>(3) x,y,z [u,v,w]</td>
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<td>(4) x,y,z [u,v,w]</td>
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<tr>
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<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td>8 z ..m</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
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<td>x,y,1/2 [0,0,w]</td>
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<tr>
<td></td>
<td>x,y,1/2 [0,0,w]</td>
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<tr>
<td>8 y ..m</td>
<td>x,y,0 [0,0,w]</td>
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<td>x,y,0 [0,0,w]</td>
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<td>1/2,1/2,z [0,v,0]</td>
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<td>1/2,1/2,z [0,v,0]</td>
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<td>4 s m'2'</td>
<td>1/2,0,z [0,v,0]</td>
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<td>1/2,0,z [0,v,0]</td>
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<td>0,0,z [0,0,0]</td>
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<td>0,y,0 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>2 g 2mm</td>
<td>0,1/2,1/2 [0,0,0]</td>
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Continued

47.6.352

2 d m'mm 1/2,0,1/2 [0,0,0]
2 c mmm 0,0,1/2 [0,0,0]
2 b m'mm 1/2,0,0 [0,0,0]
2 a mmm 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2mm1'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [0,1,0] p2mm1'  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a} \)  
Origin at 0,y,0
Origin at center (mmm)

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) +$ set

(1) $1$ $(0,0,0)$
(2) $2 \cdot 0,0,z$ $(2z,0,0,0)$
(3) $2 \cdot 0,y,0$ $(2y,0,0,0)$
(4) $2 \cdot x,0,0$ $(2x,0,0,0)$
(5) $m \cdot x,y,0$ $(m_z,0,0,0)$
(6) $m \cdot x,0,z$ $(m_y,0,0,0)$
(7) $m \cdot 0,y,z$ $(m_x,0,0,0)$
(8) $m \cdot 0,y,z$ $(m_x,0,0,0)$

For $(1,0,0)' +$ set

(1) $t' (1,0,0)$ $(1,0,0)'$
(2) $2' \cdot 1/2,0,z$ $(2z,1,0,0)'$
(3) $2' \cdot 1/2,y,0$ $(2y,1,0,0)'$
(4) $2' \cdot (1,0,0)$ $(2x,1,0,0)'$
(5) $a' (1,0,0)$ $x,y,0$ $(m_z,1,0,0)'$
(6) $a' (1,0,0)$ $x,y,0$ $(m_z,1,0,0)'$
(7) $a' (1,0,0)$ $x,0,z$ $(m_z,1,0,0)'$
(8) $m' \cdot 1/2,y,z$ $(m_x,1,0,0)'$
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<tr>
<th>Multiplicity</th>
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<td>4 q mm2</td>
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<tr>
<td>4 p m'2'm</td>
<td>1/2,y,1/2 [0,0,w]</td>
</tr>
<tr>
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<td>1/2,y,0 [0,0,w]</td>
</tr>
<tr>
<td>4 n m2m</td>
<td>0,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 m m2m</td>
<td>0,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4 l 2'm'm</td>
<td>x,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 k 2'm'm</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 j 2mm</td>
<td>x,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 i 2mm</td>
<td>x,0,0 [0,0,0]</td>
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<td>2 h m'm'm</td>
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<td>2 g mm'm</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<td>2 f m'm'm</td>
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</tr>
<tr>
<td>2 e mm'm</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Continued

47.7.353

P \text{ cmmm}

2 d' m'\text{mm} \ 1/2,0,1/2 [0,0,0]
2 c \ \text{mmm} \ 0,0,1/2 [0,0,0]
2 b' m'\text{mm} \ 1/2,0,0 [0,0,0]
2 a \ \text{mmm} \ 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] \ p\text{c'} 2\text{mm} \quad \text{Along [1,0,0]} \quad \text{p2}\text{mm1'}
\text{a} = \text{a} \quad \text{b} = \text{b}
\text{Origin at 0,0,z}
\text{Origin at x,0,0}

\text{Along [0,1,0]} \quad \text{p2}\text{mm1'}
\text{a} = \text{c} \quad \text{b} = \text{a}
Origin at center (mmm)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$
### Symmetry Operations

For \((0,0,0) +\)

\[
\begin{array}{cccc}
(1) & 1 & (2) & 2 \ 0,0,z \\
 & (1,0,0) & (2_z,0,0,0) & (2,0,0,0) \\
(5) & \bar{T} & (6) & m \ x,y,0 \\
 & (0,0,0) & (m_z,0,0,0) & (m,0,0,0) \\
(1) & t & (2) & 2' 1/2,0,z \\
 & (1,0,0) & (2_z',1,0,0) & (2,0,0,0) \\
(5) & \bar{T}' & (6) & a' (1,0,0) x,y,0 \\
 & (1,0,0)' & (m_z',1,0,0) & (m,0,0,0) \\
\end{array}
\]

For \((1,0,0)' + \)

\[
\begin{array}{cccc}
(1) & t' & (2) & 2' 1/2,0,z \\
 & (1,0,0) & (2_z',1,0,0) & (2,0,0,0) \\
(5) & \bar{T}' & (6) & a' (1,0,0) x,y,0 \\
 & (1,0,0)' & (m_z',1,0,0) & (m,0,0,0) \\
\end{array}
\]

### Generators selected

\((1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0) +)</td>
<td>((1,0,0)' +)</td>
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<tr>
<td>(\alpha 16)</td>
<td>(\alpha 16)</td>
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<tr>
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<td>(x,y,z [u,v,w])</td>
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<td>(5) (x,y,z [u,v,w])</td>
<td>(x,y,z [u,v,w])</td>
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<td>(x,y,1/2 [u,v,0])</td>
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<td>(x,y,0 [0,0,w])</td>
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<tr>
<td>(x \ .m') (x,1/2,z [u,0,w])</td>
<td>(x,1/2,z [u,0,w])</td>
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<td>(w \ .m) (x,0,z [0,v,0])</td>
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<tr>
<td>(v \ .m') (1/2,y,z [0,v,w])</td>
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</tr>
<tr>
<td>(u \ .m) (0,y,z [0,0,u])</td>
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</tr>
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<td>(2/1,0,z [0,v,0])</td>
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<td>(r \ .m') (0/1,2,z [u,0,0])</td>
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<td>(1/2,y,1/2 [0,v,0])</td>
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<td>(n \ .m') (0,y,1/2 [u,0,0])</td>
<td>(0,y,1/2 [u,0,0])</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] p2mm1'  
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [0,1,0] p2mm1'  
\[ a^* = c \quad b^* = a \]
Origin at 0,y,0
Orthorhombic

Origin at center (mmm')

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set:

1. \( \{1 \mid 0,0,0 \} \)
2. \( \{2 \mid 0,0,z \} \)
3. \( \{3' \mid 0,y,0 \} \)
4. \( \{4' \mid x,0,0 \} \)
5. \( \{5 \mid 0,0,0 \} \)
6. \( \{6 \mid m',0,0 \} \)
7. \( \{7 \mid m,0,z \} \)
8. \( \{8 \mid m,0,0 \} \)

For (1,0,0)' + set:

1. \( \{1' \mid 1,0,0 \} \)
2. \( \{2' \mid 1/2,0,z \} \)
3. \( \{3 \mid 1/2,y,0 \} \)
4. \( \{4 \mid 2(1,0,0) \} \)
5. \( \{5 \mid 1/2,0,0 \} \)
6. \( \{6 \mid a(1,0,0) \} \)
7. \( \{7 \mid a'(1,0,0) \} \)
8. \( \{8 \mid m',1/2,y,z \} \)

\( \{1 \mid 0,0,0 \} \)
\( \{2 \mid 0,0,0 \} \)
\( \{3 \mid 0,0,0 \} \)
\( \{4 \mid 0,0,0 \} \)
\( \{5 \mid 0,0,0 \} \)
\( \{6 \mid 0,0,0 \} \)
\( \{7 \mid 0,0,0 \} \)
\( \{8 \mid 0,0,0 \} \)
Continued

Generators selected \( (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5). \)

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
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<td>( 16 \alpha 1 ) x,y,z[0,v,w]</td>
<td>( x,y,z[0,v,w] )</td>
</tr>
<tr>
<td>( 8 z \ldots m' ) x,y,1/2[0,v,0]</td>
<td>( x,y,1/2[0,v,0] )</td>
</tr>
<tr>
<td>( 8 y \ldots m' ) x,y,0[0,v,0]</td>
<td>( x,y,0[0,v,0] )</td>
</tr>
<tr>
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<td>( x,1/2,z[0,v,0] )</td>
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<tr>
<td>( 8 w \ldots m ) x,0,z[0,v,0]</td>
<td>( x,0,z[0,v,0] )</td>
</tr>
<tr>
<td>( 8 v \ldots m ) 1/2,y,z[0,v,0]</td>
<td>( 1/2,y,z[0,v,0] )</td>
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<tr>
<td>( 8 u \ldots m ) 0,y,z[0,0,0]</td>
<td>( 0,y,z[0,0,0] )</td>
</tr>
<tr>
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<td>( 1/2,1/2,z[0,v,0] )</td>
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<td>( 1/2,0,z[0,v,0] )</td>
</tr>
<tr>
<td>( 4 r \ldots m ) 0,1/2,z[0,0,0]</td>
<td>( 0,1/2,z[0,0,0] )</td>
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<tr>
<td>( 4 q \ldots m ) 0,0,z[0,0,0]</td>
<td>( 0,0,z[0,0,0] )</td>
</tr>
<tr>
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<td>( 1/2,y,1/2[0,v,0] )</td>
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<td>( 0,y,1/2[0,0,0] )</td>
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<td>( 0,y,0[0,0,0] )</td>
</tr>
<tr>
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<td>( x,1/2,1/2[0,v,0] )</td>
</tr>
<tr>
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<td>( 4 j \ldots m ) x,0,1/2[0,v,0]</td>
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</tr>
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<td>( 1/2,1/2,1/2[0,v,0] )</td>
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<tr>
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<tr>
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<td>( 1/2,1/2,0[0,v,0] )</td>
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<tr>
<td>( 2 e \ldots m ) 0,1/2,0[0,0,0]</td>
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</tbody>
</table>
Continued

47.9.355

P$_2$ mmm'

2 d m'nm' 1/2,0,1/2 [0,v,0]
2 c mmm' 0,0,1/2 [0,0,0]
2 b m'nm' 1/2,0,0 [0,v,0]
2 a mmm' 0,0,0 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p$_{2a}$ 2mm</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [0,1,0]</th>
<th>p2mm1'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = c</td>
<td>b* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
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<td></td>
</tr>
</tbody>
</table>

47.9.355 - 3 - 696
Orthorhombic

47.10.356

mmm1'

P2c 2'/m'2'/m'2/m

Origin at center (mm'm')

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)

(5) 1 (1|0,0,0)

(6) m x,y,0 (mz|0,0,0)

(7) m' x,0,z (mz|0,0,0)' (7) c (0,0,1) x,0,z (mz|0,0,1)

(8) m' 0,y,z (mz|0,0,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1|0,0,1)'

(5) T 0,0,1/2 (1|0,0,1)'

(6) m' x,y,1/2 (mz|0,0,1)'

(7) c (0,0,1) x,0,z (mz|0,0,1)

(8) c (0,0,1) 0,y,z (mz|0,0,1)
Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
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<tbody>
<tr>
<td></td>
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<td></td>
<td>(0,0,1)' +</td>
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<td>16 α 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(3) x,y,z [u,v,w]</td>
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<td>(7) x,y,z [u,v,w]</td>
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<td>(8) x,y,z [u,v,w]</td>
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<tr>
<td>8 z ..m'</td>
<td>x,y,1/2 [u,v,0]</td>
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<tr>
<td>8 y ..m</td>
<td>x,y,0 [0,0,w]</td>
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<tr>
<td>8 x ..m'.</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>8 w ..m'.</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>8 v m'..</td>
<td>1/2,y,z [0,v,w]</td>
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<tr>
<td>8 u m'..</td>
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</tr>
<tr>
<td>4 t m''</td>
<td>1/2,1/2,z [0,0,w]</td>
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<tr>
<td>4 s m''</td>
<td>1/2,0,z [0,0,w]</td>
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<td>1/2,y,0 [0,0,w]</td>
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<tr>
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<td>2 g m''</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2 f m''</td>
<td>1/2,1/2,0 [0,0,w]</td>
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<tr>
<td>2 e m''</td>
<td>0,1/2,0 [0,0,w]</td>
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Continued

2 \( d \) \( m'm'm' \) 1/2,0,1/2 [0,0,0]
2 \( c \) \( m'm'm' \) 0,0,1/2 [0,0,0]
2 \( b \) \( m'm'm \) 1/2,0,0 [0,0,w]
2 \( a \) \( m'm'm \) 0,0,0 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1] \( p2mm1' \)  
\( a^* = a \) \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] \( p_{2a'}2m'm' \)  
\( a^* = -c \) \( b^* = b \)  
Origin at x,0,1/2

Along [0,1,0] \( p_{2a'}2m'm' \)  
\( a^* = c \) \( b^* = a \)  
Origin at 0,y,1/2
Origin at center (mmm')

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

**For (0,0,0) + set**

1. $1 \quad (1 \mid 0,0,0)$
2. $2 \quad 0,0,z \quad (2z \mid 0,0,0)$
3. $2' \quad 0,y,0 \quad (2z \mid 0,0,0)'$
4. $2' \quad x,0,0 \quad (2z \mid 0,0,0)'$
5. $\overline{1} \quad (1,0,0)$
6. $m' \quad x,y,0 \quad (mz \mid 0,0,0)$
7. $m \quad x,0,z \quad (mz \mid 0,0,0)$
8. $m' \quad 0,y,z \quad (mz \mid 0,0,0)$

**For (1,0,0)' + set**

1. $t' \quad (1,0,0)$
2. $2' \quad 1/2,0,z \quad (2z \mid 1,0,0)'$
3. $2 \quad 1/2,y,0 \quad (2z \mid 1,0,0)$
4. $2 \quad (1,0,0) \quad x,0,0 \quad (2z \mid 1,0,0)$
5. $\overline{1} \quad (1/2,0,0)$
6. $a \quad (1,0,0) \quad x,y,0 \quad (mz \mid 1,0,0)$
7. $a' \quad (1,0,0) \quad x,0,z \quad (mz \mid 1,0,0)'$
8. $m' \quad 1/2,y,z \quad (mz \mid 1,0,0)'$
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<tr>
<td>8 v m'</td>
<td>1/2,y,z [u,0,0]</td>
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</tr>
<tr>
<td>4 p m'2'</td>
<td>1/2,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 o m'2'</td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 n m'2'</td>
<td>0,y,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 m m'2'</td>
<td>0,y,0 [u,0,0]</td>
</tr>
<tr>
<td>4 l m'2'</td>
<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 k m'2'</td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 j m'2'</td>
<td>x,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 i m'2'</td>
<td>x,0,0 [0,v,0]</td>
</tr>
<tr>
<td>2 h m'2m'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 g m'2m'</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 f m'2m'</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 e m'2m'</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
</tbody>
</table>
Continued

<table>
<thead>
<tr>
<th>2</th>
<th>d</th>
<th>m' mm'</th>
<th>1/2, 0, 1/2</th>
<th>[0, v, 0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>c</td>
<td>mmm'</td>
<td>0, 0, 1/2</td>
<td>[0, 0, 0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>m' mm'</td>
<td>1/2, 0, 0</td>
<td>[0, v, 0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>mmm'</td>
<td>0, 0, 0</td>
<td>[0, 0, 0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0, 0, 1]</th>
<th>p_c 2mm</th>
<th>Along [1, 0, 0]</th>
<th>p2mm1'</th>
<th>Along [0, 1, 0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a</td>
<td>b' = b</td>
<td>a' = b</td>
<td>b' = c</td>
<td>a' = c</td>
<td>b' = a</td>
</tr>
<tr>
<td>Origin at 0, 0, z</td>
<td></td>
<td>Origin at x, 0, 0</td>
<td></td>
<td>Origin at 0, y, 0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin**  at 222, at 1/4,1/4,1/4 from \( \bar{1} \)

**Asymmetric unit**  

\( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)

**Symmetry Operations**

1. \( \bar{1} \)
   
   \begin{align*}
   (1,0,0,0) \\
   (1,0,0,0)
   \end{align*}

2. \( \bar{2} \)
   
   \begin{align*}
   (0,0,z) \\
   (2z,0,0,0)
   \end{align*}

3. \( \bar{2} \)
   
   \begin{align*}
   (0,y,0) \\
   (2y,0,0,0)
   \end{align*}

4. \( \bar{2} \)
   
   \begin{align*}
   (x,0,0) \\
   (2x,0,0,0)
   \end{align*}

5. \( \bar{1} \)
   
   \begin{align*}
   (1/4,1/4,1/4) \\
   (1/2,1/2,1/2)
   \end{align*}

6. \( \bar{n} \)
   
   \begin{align*}
   (1/2,1/2,0) \\
   (m_x,1/2,1/2,1/2)
   \end{align*}

7. \( \bar{n} \)
   
   \begin{align*}
   (1/2,0,1/2) \\
   (m_y,1/2,1/2,1/2)
   \end{align*}

8. \( \bar{n} \)
   
   \begin{align*}
   (0,1/2,1/2) \\
   (m_z,1/2,1/2,1/2)
   \end{align*}
Generators selected: 
(1) t(1,0,0); t(0,1,0); t(0,0,1); (2) (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 l 1/2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 k 1/2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 j 1/2</td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 i 1/2</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 h 1/2</td>
<td>X,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 g 1/2</td>
<td>X,0,0 [u,0,0]</td>
</tr>
<tr>
<td>4 f 1/2</td>
<td>3/4,3/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td>4 e 1/2</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td>2 d 1/2</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 c 1/2</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 1/2</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 1/2</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c_p 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c_p 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = b</td>
<td>b^* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>c_p 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = c</td>
<td>b^* = a</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
**Orthorhombic**

**Pnnn1'**

48.2.359

**mmm1'**

P2/n2/n2/n1'

**1'**

Origin: at 2221', at 1/4,1/4,1/4 from 1

Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

**Symmetry Operations**

For 1 + set

1. \(T\) \((0,0,0)
2. \(2\) \((0,0,z)\)
3. \(2\) \((0,y,0)\)
4. \(2\) \((x,0,0)\)
5. \(1\) \((1/4,1/4,1/4)\)
6. \(n\) \((1/2,1/2,0)\)
7. \(n\) \((1/2,0,1/2)\)
8. \(n\) \((0,1/2,1/2)\)

For 1' + set

1. \(T\) \((0,0,0)'\)
2. \(2\) \((0,0,z)\)
3. \(2\) \((0,y,0)\)
4. \(2\) \((x,0,0)\)
5. \(1\) \((1/4,1/4,1/4)\)
6. \(n\) \((1/2,1/2,0)\)
7. \(n\) \((1/2,0,1/2)\)
8. \(n\) \((0,1/2,1/2)\)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5), 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 m 11' (1) x,y,z [0,0,0]</td>
<td>(2) x̅,y̅,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) x̅,y̅,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x̅,y̅,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

4 l .21' 0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 1/2,0,z+1/2 [0,0,0] 1/2,0,z+1/2 [0,0,0]
4 k .21' 0,0,z [0,0,0] 0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 1/2,1/2,z+1/2 [0,0,0]
4 j .21' 1/2,y,0 [0,0,0] 1/2,y,0 [0,0,0] 0,y+1/2,1/2 [0,0,0] 0,y+1/2,1/2 [0,0,0]
4 i .21' 0,y,0 [0,0,0] 0,y,0 [0,0,0] 1/2,y+1/2,1/2 [0,0,0] 1/2,y+1/2,1/2 [0,0,0]
4 h .21' x,0,1/2 [0,0,0] x̅,0,1/2 [0,0,0] x+1/2,1/2,0 [0,0,0] x+1/2,1/2,0 [0,0,0]
4 g .21' x,0,0 [0,0,0] x̅,0,0 [0,0,0] x+1/2,1/2,1/2 [0,0,0] x+1/2,1/2,1/2 [0,0,0]
4 f .1' 3/4,3/4,3/4 [0,0,0] 1/4,1/4,3/4 [0,0,0] 1/4,3/4,1/4 [0,0,0] 3/4,1/4,1/4 [0,0,0]
4 e .1' 1/4,1/4,1/4 [0,0,0] 3/4,3/4,1/4 [0,0,0] 3/4,1/4,3/4 [0,0,0] 1/4,3/4,3/4 [0,0,0]
2 d 2221' 0,1/2,0 [0,0,0] 1/2,0,1/2 [0,0,0]
2 c 2221' 0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]
2 b 2221' 1/2,0,0 [0,0,0] 0,1/2,1/2 [0,0,0]
2 a 2221' 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] c 2mm1'</th>
<th>Along [1,0,0] c 2mm1'</th>
<th>Along [0,1,0] c 2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = c b* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin at \(22'2', 1/4,1/4,1/4\) from \(\overline{1}\)

Asymmetric unit \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

(1) \(1 \quad (1' | 0,0,0)\)

(2) \(2' \quad 0,0,z \quad (2z' | 0,0,0)\)

(3) \(2' \quad 0,y,0 \quad (2y' | 0,0,0)\)

(4) \(2 \quad x,0,0 \quad (2x' | 0,0,0)\)

(5) \(\overline{1'} \quad 1/4,1/4,1/4 \quad (\overline{1'} | 1/2,1/2,1/2)\)

(6) \(n \quad (1/2,1/2,0) \quad x,y,1/4 \quad (mz | 1/2,1/2,1/2)\)

(7) \(n \quad (1/2,0,1/2) \quad x,1/4,z \quad (mx | 1/2,1/2,1/2)\)

(8) \(n' \quad (0,1/2,1/2) \quad 1/4,y,z \quad (mz' | 1/2,1/2,1/2)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 l .2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 k .2'</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 j .2'</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y+1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y+1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 i .1'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y+1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y+1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 h 2..</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 g 2..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 f 1..</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/4,1/4,3/4 [0,0,0]</td>
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<td>1/4,1/4,3/4 [0,0,0]</td>
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<tr>
<td>4 e 1..</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
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<td></td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 d 22'2'</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 c 22'2'</td>
<td>0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>2 b 22'2'</td>
<td>1/2,0,0 [u,0,0]</td>
</tr>
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<td>0,1/2,0 [u,0,0]</td>
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<tr>
<td>2 a 22'2'</td>
<td>0,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c p 2mm' c p 2mm' c p 2mm'  
\( a^* = a \) \( b^* = b \)  \( a^* = b \) \( b^* = c \)  \( a^* = -a \) \( b^* = c \)  
Origin at 0,0,0  Origin at x,0,0  Origin at 0,0,0  

48.3.360 - 2 - 708
Origin at $2'2'2'$, at $1/4,1/4,1/4$ from $\overline{1}$

Asymmetric unit $0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1$

Symmetry Operations

(1) 1
(1 0,0,0)

(2) $2\ 0,0,z$
($2_z\ 0,0,0$)

(3) $2'\ 0,y,0$
($2'_{x,0,0}$)

(4) $2'\ x,0,0$
($2'_{x,0,0}$)

(5) $\overline{1}\ 1/4,1/4,1/4$
($\overline{1}\ 1/2,1/2,1/2$)

(6) $n\ (1/2,1/2,0)\ x,y,1/4$
($m_{z}\ 1/2,1/2,1/2$)

(7) $n'\ (1/2,0,1/2)\ x,1/4,z$
($m_{y}\ 1/2,1/2,1/2'$)

(8) $n'\ (0,1/2,1/2)\ 1/4,y,z$
($m_{x}\ 1/2,1/2,1/2'$)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

| 4 l .2   | 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] |
| 4 k ..2  | 0,0,z [0,0,w] 0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w] |
| 4 j .2'  | 1/2,y,0 [u,0,w] 1/2,y,0 [u,0,w] 0,y+1/2,1/2 [u,0,w] 0,y+1/2,1/2 [u,0,w] |
| 4 i .2'  | 0,y,0 [u,0,w] 0,y,0 [u,0,w] 1/2,y+1/2,1/2 [u,0,w] 1/2,y+1/2,1/2 [u,0,w] |
| 4 h 2'.. | X,0,1/2 [0,v,w] X,0,1/2 [0,v,w] x+1/2,1/2,0 [0,v,w] x+1/2,1/2,0 [0,v,w] |
| 4 g 2'.. | X,0,0 [0,v,w] X,0,0 [0,v,w] x+1/2,1/2,1/2 [0,v,w] x+1/2,1/2,1/2 [0,v,w] |
| 4 e 1    | 1/4,1/4,1/4 [u,v,w] 3/4,1/4,1/4 [u,v,w] 3/4,1/4,1/4 [u,v,w] 1/4,3/4,3/4 [u,v,w] |
| 2 d 2'2' | 0,1/2,0 [0,0,w] 1/2,0,1/2 [0,0,w] |
| 2 c 2'2' | 0,0,1/2 [0,0,w] 1/2,1/2,0 [0,0,w] |
| 2 b 2'2' | 1/2,0,0 [0,0,w] 0,1/2,1/2 [0,0,w] |
| 2 a 2'2' | 0,0,0 [0,0,w] 1/2,1/2,1/2 [0,0,w] |

Symmetry of Special Projections

Along [0,0,1] c2m'm'  Along [1,0,0] c 2'mm'  Along [0,1,0] c 2'mm'

a'^* = a  b'^* = b  a'^* = -c  b'^* = b  a'^* = c  b'^* = a

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Orthorhombic

Pn'n'n'  48.5.362

m'm'm'  P2/n'2/n'2/n'

Origin  at 222, at 1/4,1/4,1/4 from \( \overline{1} \)

Asymmetric unit  0 ≤ x ≤ 1/4;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1 & \quad 0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2 & \quad z,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(2 & \quad y,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(2 & \quad x,0,0) \\
(5) & \quad \overline{1} \quad 1/4,1/4,1/4 \\
(\overline{1} & \quad 1/2,1/2,1/2) \\
(6) & \quad n' \quad (1/2,1/2,0) \quad x,y,1/4 \\
(m_z & \quad 1/2,1/2,1/2) \\
(7) & \quad n' \quad (1/2,0,1/2) \quad x,1/4,z \\
(m_y & \quad 1/2,1/2,1/2) \\
(8) & \quad n' \quad (0,1/2,1/2) \quad 1/4,y,z \\
(m_z & \quad 1/2,1/2,1/2) \\
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) m 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) m 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) m 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(4) m 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) m 1</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(6) m 1</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(7) m 1</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(8) m 1</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c 2m'm'  
Along [0,1,0] c 2m'm'  
Along [1,0,0] c 2m'm'

a* = a  b* = b  
a* = b  b* = c  
a* = c  b* = a

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin  at 222, at 1/4,1/4,1/4 from 1
Asymmetric unit  0 ≤ x ≤ 1/4;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1

48.6.363 - 1 - 713
Continued

### Symmetry Operations

<table>
<thead>
<tr>
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<th>For (0,0,0) + set</th>
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<tbody>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2 ( \end{equation}^{0,0,0} )</td>
</tr>
<tr>
<td>3</td>
<td>2 ( \end{equation}^{0,0,0} )</td>
</tr>
<tr>
<td>4</td>
<td>2 ( \end{equation}^{x,0,0} )</td>
</tr>
<tr>
<td>5</td>
<td>( \setminus ) ( 1/4,1,1/4 ) ( \setminus ) ( 1,1/2,1/2 )</td>
</tr>
<tr>
<td>6</td>
<td>( n ) ( (1/2,1/2,0) ) ( x,y,1/4 )</td>
</tr>
<tr>
<td>7</td>
<td>( n ) ( (1/2,0,1/2) ) ( x,1/4,z )</td>
</tr>
<tr>
<td>8</td>
<td>( n ) ( (0,1,2/1) ) ( 1/4,y,z )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>For (1,0,0)′ + set</th>
</tr>
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<tr>
<td>1</td>
<td>( t ) ( (1,0,0) )</td>
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<td>2</td>
<td>( t ) ( (0,1,0) )</td>
</tr>
<tr>
<td>3</td>
<td>( t ) ( (0,0,1) )</td>
</tr>
<tr>
<td>4</td>
<td>( t ) ( (1,1,0) )</td>
</tr>
<tr>
<td>5</td>
<td>( n ) ( (1/2,1/2,0) ) ( x,y,1/4 )</td>
</tr>
<tr>
<td>6</td>
<td>( n ) ( (1/2,0,1/2) ) ( x,1/4,z )</td>
</tr>
<tr>
<td>7</td>
<td>( n ) ( (0,1,2/1) ) ( 3/4,y,z )</td>
</tr>
</tbody>
</table>

Generators selected  
(1); \( t \)′(1,0,0); \( t \)′(0,1,0); \( t \)′(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th></th>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>16 m 1</td>
<td>((0,0,0) + ) (1,0,0)′ +</td>
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<tr>
<td></td>
<td>( x,y,z [u,v,w] )</td>
<td>( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>( x,y,z [u,v,w] )</td>
<td>( x,y,z [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>( x+1/2,y+1/2,z+1/2 [u,v,w] )</td>
<td>( x+1/2,y+1/2,z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>( x+1/2,y+1/2,z+1/2 [u,v,w] )</td>
<td>( x+1/2,y+1/2,z+1/2 [u,v,w] )</td>
</tr>
<tr>
<td>8</td>
<td>l ( ..2 ) 0,1/2,2 [0,0,w]</td>
<td>0,1/2,2 [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>k ( ..2 ) 0,0,2 [0,0,w]</td>
<td>0,0,2 [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>j ( ..2 ) 1/2,1/2 [0,0,w]</td>
<td>1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>i ( ..2 ) 0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>h ( ..2 ) 1/2,1/2 [0,0,0]</td>
<td>1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>g ( ..2 ) 0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>f ( \bar{1} ) 3/4,3/4,3/4 [u,v,w]</td>
<td>3/4,3/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td>8</td>
<td>e ( \bar{1} ) 1/4,1/4,1/4 [u,v,w]</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>d ( 222 ) 0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c ( 222 ) 0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b ( 222 ) 0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>
4  a  222  0,0,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  c2mm1'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0]  c2mm1'  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [0,1,0]  c2mm1'  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a} \)  
Origin at 0,y,0
**Orthorhombic**

**49.1.364**

**Pccm**

Origin at center (2/m) at cc2/m

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

1. 1 (1 | 0, 0, 0)
2. 2 | 0, 0, z
   (2 | 0, 0, 0)
3. 2 | 0, y, 1/4
   (2 | 0, 0, 1/2)
4. 2 | x, 0, 1/4
   (2 | 0, 0, 1/2)
5. m (1 | 0, 0, 0)
6. m | x, y, 0
   (m | 0, 0, 0)
7. c (0, 0, 1/2) | x, 0, z
   (m | 0, 0, 1/2)
8. c (0, 0, 1/2) | 0, y, z
   (m | 0, 0, 1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 r 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(8) x,y,z+1/2 [u,v,w]</td>
<td>(9) x,y,z [u,v,w]</td>
<td>(10) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 q ..m x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 p ..2 1/2,0,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>4 o ..2 0,1/2,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 n ..2 1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 m ..2 0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
</tr>
<tr>
<td>4 l 1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 k 2 ... x,1/2,1/4 [u,0,0]</td>
<td>x,1/2,1/4 [u,0,0]</td>
<td>x,1/2,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 j 2 ... x,0,1/4 [u,0,0]</td>
<td>x,0,1/4 [u,0,0]</td>
<td>x,0,1/4 [u,0,0]</td>
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<tr>
<td>2 h 222 1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
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<tr>
<td>2 g 222 0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
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<tr>
<td>2 f 222 1/2,0,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
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<tr>
<td>2 e 222 0,0,1/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2 d ..2/m 1/2,0,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2 c ..2/m 0,1/2,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 b ..2/m 1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
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<tr>
<td>2 a ..2/m 0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Along [0,0,1]</th>
<th>p2mm1'</th>
<th>Along [1,0,0]</th>
<th>p_{2\alpha} 2m'm'</th>
<th>Along [0,1,0]</th>
<th>p_{2\alpha} 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a  b* = b</td>
<td>a* = c/2</td>
<td>b* = b</td>
<td>a* = c/2</td>
<td>b* = a</td>
<td>a* = c/2</td>
<td>b* = a</td>
</tr>
</tbody>
</table>

Origin at 0,0,z | Origin at x,0,0 | Origin at 0,y,0
Origin at center (2/m1') at cc2/m1'

Asymmetric unit
0 < x < 1/2; 0 < y < 1/2; 0 < z < 1/2

Symmetry Operations

For 1 + set
(1) 1
   (1' | 0,0,0)
   (1 | 0,0,0)
(2) 2  0,0,z
   (2_ | 0,0,0)
   (2_ | 0,0,0)
(3) 2  y,1/4
   (2_y | 0,0,1/2)
   (2_y | 0,0,1/2)
(4) 2  x,0,1/4
   (2_x | 0,0,1/2)
   (2_x | 0,0,1/2)

For 1' + set
(5) 1'
    (5' | 0,0,0)
    (1' | 0,0,0)
(6)  m  x,y,0
    (6' | m_0,0,0)
    (6' | m_0,0,0)
(7)  c  (0,0,1/2)  x,0,z
    (7' | c_0,0,1/2')  x,0,z
    (7' | c_0,0,1/2')  x,0,z
(8)  c  (0,0,1/2)  0,y,z
    (8' | c_0,0,1/2')  0,y,z
    (8' | c_0,0,1/2')  0,y,z
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coordinates</td>
</tr>
<tr>
<td>-----------------</td>
</tr>
<tr>
<td>8 r 11'</td>
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<tr>
<td>(5) x, y, z [0, 0, 0]</td>
</tr>
<tr>
<td>4 q ..m1'</td>
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<tr>
<td>4 p ..21'</td>
</tr>
<tr>
<td>4 o ..21'</td>
</tr>
<tr>
<td>4 n ..21'</td>
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<tr>
<td>4 m ..21'</td>
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<td>4 l ..2.1'</td>
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<td>4 k ..2.1'</td>
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<tr>
<td>4 j ..2.1'</td>
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<td>2 h 2221'</td>
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<td>2 e 2221'</td>
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<td>2 d ..2/m1'</td>
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<tr>
<td>2 c ..2/m1'</td>
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<tr>
<td>2 b ..2/m1'</td>
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<tr>
<td>2 a ..2/m1'</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1' Along [1,0,0] p2mm1' Along [0,1,0] p2mm1'

\[ a^* = a \quad b^* = b \]
\[ a^* = b \quad b^* = c/2 \]
\[ a^* = c/2 \quad b^* = a \]
**Origin**  
at center (2'/m ) at c'c2'/m

**Asymmetric unit**  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

- (1) 1  
  (1 | 0,0,0)

- (2) 2'  
  (2' | 0,0,0)
  (2' | 0,0,1/2)

- (3) 2'  
  (2' | 0,0,1/2)
  (2' | 0,0,1/2)

- (4) 2  
  (2 | 0,0,1/2)
  (2 | 0,0,1/2)

- (5) T'  
  (T | 0,0,0)

- (6) m  
  (m | x,y,0)
  (m | 0,0,0)

- (7) c  
  (c | 0,0,1/2)
  (m | 0,0,1/2)

- (8) c'  
  (c' | 0,0,1/2)
  (m | 0,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

**Multiplicities, Wyckoff Letters, Site Symmetries**

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>8</td>
<td>r</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
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<tr>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2 a 2'</td>
<td>0,0,0 [0,0,0]</td>
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<td>a</td>
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<td>0,0,0 [0,0,0]</td>
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<td>0,0,1/2 [0,0,0]</td>
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</table>

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
Along [1,0,0] p 2mm  
Along [0,1,0] p 2mm'  
\( \mathbf{a}^* = \mathbf{a} \)  
\( \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z  
Origin at x,0,0

\( \mathbf{a}^* = \mathbf{b} \)  
\( \mathbf{b}^* = c/2 \)  
Origin at 0,0,z  
Origin at x,0,0

\( \mathbf{a}^* = c/2 \)  
\( \mathbf{b}^* = \mathbf{a} \)  
Origin at 0,y,0  
Origin at 0,0,z
Origin at center (2/m') at cc2/m'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1 (1|0,0,0)  
(2) 2  0,0,0  (2_z|0,0,0)  
(3) 2'  0,y,1/4  (2|0,0,1/2)'
(4) 2'  x,0,1/4  (2_z|0,0,1/2)'

(5) \( \bar{1} \)  (0|0,0,0)'
(6) m'  x,y,0  (m_z|0,0,0)'
(7) c  (0,0,1/2)  x,0,z  (m|0,0,1/2)
(8) c  (0,0,1/2)  0,y,z  (m_z|0,0,1/2)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Continued

Coordinates

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<tr>
<td>8 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td>4 q .m'</td>
<td>x,y,0 [u,v,0]</td>
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<td>x,y,1/2 [u,v,0]</td>
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<td>1/2,y,1/4 [u,0,w]</td>
<td>1/2,y,1/4 [u,0,w]</td>
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<td>0,y,1/4 [u,0,w]</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,1/4 [u,0,w]</td>
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<td>2 c .2/m'</td>
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Symmetry of Special Projections

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<th>p2mm</th>
<th>Along [1,0,0]</th>
<th>p2e' 2'mm'</th>
<th>Along [0,1,0]</th>
<th>p2e' 2'mm'</th>
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<td></td>
<td>a* = -c/2</td>
<td>b* = b</td>
<td>a* = c/2</td>
<td>b* = a</td>
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<td>Origin at x,0,0</td>
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<td>Origin at 0,y,0</td>
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Pc’c’m
49.5.368

m’m’m
P2’/c’2’/c’2/m

Orthorhombic

Origin  at center ( 2/m ) at c’c’2/m

Asymmetric unit  0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
     (1 | 0,0,0)

(2) 2 0,0,z
     (2 | 0,0,0)

(3) 2’ 0,y,1/4
     (2 | 0,0,1/2)’

(4) 2’ x,0,1/4
     (2 | 0,0,1/2)’

(5) 1
     (1 | 0,0,0)

(6) m x,y,0
     (m | 0,0,0)

(7) c’ (0,0,1/2) x,0,z
     (m | 0,0,1/2)’

(8) c’ (0,0,1/2) 0,y,z
     (m | 0,0,1/2)’
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions  Coordinates
Multiplicity, Wyckoff letter, Site Symmetry.

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<th>(3) x,y,z+1/2 [u,v,w]</th>
<th>(4) x,y,z+1/2 [u,v,w]</th>
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<tr>
<td>4 l</td>
<td>.2'</td>
<td>1/2,y,1/4 [0,0,w]</td>
<td>1/2,y,1/4 [0,0,w]</td>
<td>1/2,y,3/4 [0,0,w]</td>
<td>1/2,y,3/4 [0,0,w]</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>4 k</td>
<td>.2'</td>
<td>0,y,1/4 [0,0,w]</td>
<td>0,y,1/4 [0,0,w]</td>
<td>0,y,3/4 [0,0,w]</td>
<td>0,y,3/4 [0,0,w]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 j</td>
<td>2'..</td>
<td>x,1/2,1/4 [0,v,w]</td>
<td>x,1/2,1/4 [0,v,w]</td>
<td>x,1/2,3/4 [0,v,w]</td>
<td>x,1/2,3/4 [0,v,w]</td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 i</td>
<td>2'..</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,3/4 [0,v,w]</td>
<td>x,0,3/4 [0,v,w]</td>
<td></td>
<td></td>
<td></td>
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</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] p2mm1'  Along [1,0,0] p2mm  Along [0,1,0] p 2m'm'
\( a^* = a \)  \( b^* = b \)  \( a^* = c/2 \)  \( b^* = a \)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
### Symmetry Operations

1. $I \quad (1; 0,0,0)$
2. $2' \quad 0,0,z \quad (2_z; 0,0,0)'$
3. $2 \quad 0,y,1/4 \quad (2_z; 0,0,1/2)$
4. $2' \quad x,0,1/4 \quad (2_z; 0,0,1/2)'$
5. $I' \quad (1; 0,0,0)$
6. $m' \quad x,y,0 \quad (m_z; 0,0,0)'$
7. $c \quad (0,0,1/2) \quad x,0,z \quad (m_y; 0,0,1/2)$
8. $c' \quad (0,0,1/2) \quad 0,y,z \quad (m_z; 0,0,1/2)'$

### Asymmetric Unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$
Generators selected  (1); (1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 q ..m'</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>4 p ..2'</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 o ..2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 n ..2'</td>
<td>1/2,1/2,z [u,v,0]</td>
<td>1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 m ..2'</td>
<td>0,0,z [u,v,0]</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 l ..2.</td>
<td>1/2,1/4 [0,v,0]</td>
<td>1/2,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 k ..2.</td>
<td>0,y,1/4 [0,v,0]</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 j ..2'</td>
<td>x,1/2,1/4 [0,v,w]</td>
<td>x,1/2,1/4 [0,v,w]</td>
</tr>
<tr>
<td>4 i ..2'</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>2 h 2'22'</td>
<td>1/2,1/2,1/4 [0,v,0]</td>
<td>1/2,1/2,1/4 [0,v,0]</td>
</tr>
<tr>
<td>2 g 2'22'</td>
<td>0,1/2,1/4 [0,v,0]</td>
<td>0,1/2,1/4 [0,v,0]</td>
</tr>
<tr>
<td>2 f 2'22'</td>
<td>1/2,0,1/4 [0,v,0]</td>
<td>1/2,0,1/4 [0,v,0]</td>
</tr>
<tr>
<td>2 e 2'22'</td>
<td>0,0,1/4 [0,v,0]</td>
<td>0,0,1/4 [0,v,0]</td>
</tr>
<tr>
<td>2 d ..2'm'</td>
<td>1/2,0,0 [u,v,0]</td>
<td>1/2,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2 c ..2'm'</td>
<td>0,1/2,0 [u,v,0]</td>
<td>0,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2 b ..2'm'</td>
<td>1/2,1/2,0 [u,v,0]</td>
<td>1/2,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2 a ..2'm'</td>
<td>0,0,0 [u,v,0]</td>
<td>0,0,1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2'2mm'</th>
<th>Along [1,0,0]</th>
<th>p2'2mm'</th>
<th>Along [0,1,0]</th>
<th>p2z 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b b* = a</td>
<td>a* = b b* = -c/2</td>
<td>a* = c/2 b* = a</td>
<td>a* = c/2 b* = a</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,0,0

Origin at 0,y,0
Pc'c'm'  
49.7.370

m'm'm'  
P2/c'2/c'2/m'

**Orthorhombic**

**Origin**  
at center (2/m') at c'c'2/m'

**Asymmetric unit**  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

1. 1  
(1|0,0,0)

2. 2 0,0,z  
(2z|0,0,0)

3. 2 0,y,1/4  
(2y|0,0,1/2)

4. 2 x,0,1/4  
(2x|0,0,1/2)

5. 1'  
(1|0,0,0)'

6. m' x,y,0  
(mz|0,0,0)'

7. c' (0,0,1/2)  x,0,z  
(m|0,0,1/2)'

8. c' (0,0,1/2)  0,y,z  
(m|0,0,1/2)'
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 r 1 (1) x,y,z [u,v,w]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>x,1/2,3/4 [u,0,0]</td>
</tr>
<tr>
<td>4 q ..m' x,y,0 [u,v,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 p ..2 1/2,0,z [0,0,w]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 o ..2 0,1/2,z [0,0,w]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 n ..2 1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 m ..2 0,0,z [0,0,w]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2m'm'</th>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
<th>Along [0,1,0]</th>
<th>p2m'm'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c/2</td>
<td>a* = c/2</td>
<td>b* = a</td>
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<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,0,0</td>
<td>Origin at 0,x,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin  at center (2/m) at cc2/m

Asymmetric unit  0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2|0,0,0)

(3) 2 0,y,1/4
(2|0,0,1/2)

(4) 2 x,0,1/4
(2|0,0,1/2)

(5) m x,y,0
(m|0,0,0)

(6) m z 1/2,0,z
(m|0,0,1/2)

(7) c (0,0,1/2) x,0,z
(m|0,0,1/2)

(8) c (0,0,1/2) 0,y,z
(m|0,0,1/2)

For (1,0,0)’ + set

(1) t’ (1,0,0)
(1|1,0,0)’

(2) 2’ 1/2,0,z
(2|1,0,0)’

(3) 2’ 1/2,y,1/4
(2|1,0,1/2)’

(4) 2’ x,0,1/4
(2|1,0,1/2)’

(5) t’ 1/2,0,0
(1|1,0,0)’

(6) a’ (1,0,0) x,y,0
(a|1,0,0)’

(7) n’ (1,0,1/2) x,0,z
(n|1,0,1/2)’

(8) c’ (0,0,1/2) 1/2,y,z
(c|1,0,1/2)’
Generators selected
(1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16 r 1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) x,y,z+1/2 [u,v,w]</th>
<th>(4) x,y,z+1/2 [u,v,w]</th>
<th>(5) x,y,z [u,v,w]</th>
<th>(6) x,y,z [u,v,w]</th>
<th>(7) x,y,z+1/2 [u,v,w]</th>
<th>(8) x,y,z+1/2 [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 q ...m</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,1/2 [0,0,w]</td>
<td>x,y,1/2 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,1/2 [0,0,w]</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 p ...2'</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,0,z+1/2 [u,v,0]</td>
<td>1/2,0,z+1/2 [u,v,0]</td>
<td>1/2,0,z+1/2 [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
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<td>1/2,0,z+1/2 [u,v,0]</td>
<td>1/2,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 o ...2</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
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<td>0,1/2,z+1/2 [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 n ...2'</td>
<td>1/2,1/2,z [u,v,0]</td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
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<td>1/2,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 m ...2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 l ...2'</td>
<td>1/2,1/4 [0,0,w]</td>
<td>1/2,1/4 [0,0,w]</td>
<td>1/2,1/4 [0,0,w]</td>
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</tr>
<tr>
<td>8 k ...2</td>
<td>0,y,1/4 [0,v,0]</td>
<td>0,y,3/4 [0,v,0]</td>
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</tr>
<tr>
<td>8 j ...2</td>
<td>x,1/2,1/4 [u,0,0]</td>
<td>x,1/2,3/4 [u,0,0]</td>
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<td>x,1/2,3/4 [u,0,0]</td>
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<tr>
<td>8 i ...2</td>
<td>x,0,1/4 [u,0,0]</td>
<td>x,0,3/4 [u,0,0]</td>
<td>x,0,3/4 [u,0,0]</td>
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<td>x,0,1/4 [u,0,0]</td>
<td>x,0,1/4 [u,0,0]</td>
<td>x,0,3/4 [u,0,0]</td>
<td>x,0,3/4 [u,0,0]</td>
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<tr>
<td>4 h 222</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
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<tr>
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<td>0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
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<td>0,1/2,3/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
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<tr>
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<td>1/2,0,3/4 [0,0,0]</td>
<td>1/2,0,3/4 [0,0,0]</td>
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</tr>
<tr>
<td>4 e 222</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
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<td>0,0,3/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
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<tr>
<td>4 d ...2'm</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
<td>4 c ...2'm</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<td>4 b ...2'm</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a ...2'm</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p 2mm1'
Along [0,1,0] p 2mm1'
Along [0,1,0] p 2mm1'

\(a^* = a\) \(b^* = b\)
\(a^* = b\) \(b^* = c/2\)
\(a^* = -a\) \(b^* = c/2\)

Origin at 0,0,z
Origin at x,0,0
Origin at 0,y,0

49.8.371 - 2 - 731
Origin at center (2/m) at cc2/m

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) \( \bar{1} \) (0,0,0)
(2) \( 2 \) 0,0,z
(3) \( 2 \) 0,y,1/4
(4) \( 2 \) x,0,1/4

For (1,0,0)' + set

(5) \( \bar{1} \) (1,0,0)
(6) m x,y,0
(7) c (0,0,1/2) x,0,z
(8) c (0,0,1/2) 0,y,z

49.9.372 - 1 - 732
Generators selected (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) +</td>
<td>(1,0,0)* +</td>
</tr>
<tr>
<td>16 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 q .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 p .2'</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 o .2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>8 n .2</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 m .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 l .2'.</td>
<td>1/2,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 k .2.</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 j .2'.</td>
<td>x,1/2,1/4 [0,v,w]</td>
</tr>
<tr>
<td>8 i .2.</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 h 2'2'</td>
<td>1/2,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 g 2'2'</td>
<td>0,1/2,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 f 2'2'</td>
<td>1/2,0,1/4 [0,u,0]</td>
</tr>
<tr>
<td>4 e 22'</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 d .2'2'm</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2'2'm</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b .2'm</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 a .2'm</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1'  
 Along [1,0,0] p2mm1'  
 Along [0,1,0] p2mm1'

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

\[ a^* = b \quad b^* = c/2 \]

Origin at x,0,0

\[ a^* = c/2 \quad b^* = a \]

Origin at 0,y,0
$P_2a\ ccm'$

$mmm1'$

Orthorhombic

$49.10.373$

$P_{2a}\ 2'/c2'/c2/m'$

Origin at center (2/m') at cc2/m'

Asymmetric unit

$0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2|0,0,0)

(3) 2' 0,y,1/4
(2'|0,0,1/2)

(4) 2' x,0,1/4
(2'|0,0,1/2)

(5) m' x,y,0
(m|0,0,0)

(1*0,0,0)

(6) m' x,y,0
(m|0,0,0)

(1*0,0,0)

(7) c (0,0,1/2) x,0,z
(c|0,0,1/2)

(8) c (0,0,1/2) 0,y,z
(c|0,0,1/2)

For (1,0,0)' + set

(1) t' (1,0,0)
(1|1,0,0)

(2) 2' 1/2,0,z
(2'|1,0,0)

(3) 2 1/2,y,1/4
(2|1,0,1/2)

(4) 2 (1,0,0) x,0,1/4
(2|1,0,1/2)

(5) 1/2,2,0,0
(1|1,0,0)

(6) a (1,0,0) x,y,0
(m|1,0,0)

(7) n' (1,0,1/2) x,0,z
(m|1,0,1/2)

(8) c' (0,0,1/2) 1/2,y,z
(m|1,0,1/2)
Generators selected  

\( (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5). \)

**Positions**

Multiplicity,
Wyckoff letter,
Site Symmetry.

\[
\begin{array}{cccc}
\text{Position} & \text{Multiplicity} & \text{Wyckoff Letter} & \text{Site Symmetry} \\
(0,0,0) + & (1,0,0)' + & \\
16 & r & 1 & (1) x,y,z [u,v,w] \\
& & & (2) \bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}] \\
& & & (3) x,\bar{y},\bar{z}+1/2 [u,v,w] \\
& & & (4) x,\bar{y},\bar{z}+1/2 [u,v,w] \\
& & & (5) \bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}] \\
8 & q & .m' & x,y,0 [u,v,0] \\
& & & \bar{x},\bar{y},0 [\bar{u},\bar{v},0] \\
& & & \bar{x},y,1/2 [\bar{u},v,0] \\
& & & x,y,1/2 [u,v,0] \\
8 & p & .2' & 1/2,0,z [u,v,0] \\
& & & 1/2,0,\bar{z}+1/2 [u,v,0] \\
& & & 1/2,0,\bar{z}+1/2 [u,v,0] \\
8 & o & .2 & 0,1/2,z [0,0,w] \\
& & & 0,1/2,\bar{z}+1/2 [0,0,w] \\
& & & 0,1/2,\bar{z}+1/2 [0,0,w] \\
8 & n & .2' & 1/2,1/2,z [u,v,0] \\
& & & 1/2,1/2,\bar{z}+1/2 [\bar{u},\bar{v},0] \\
& & & 1/2,1/2,\bar{z}+1/2 [\bar{u},\bar{v},0] \\
8 & m & .2 & 0,0,z [0,0,w] \\
& & & 0,0,\bar{z}+1/2 [0,0,\bar{w}] \\
& & & 0,0,\bar{z}+1/2 [0,0,\bar{w}] \\
8 & l & .2 & 1/2,y,1/4 [u,v,0] \\
& & & 1/2,\bar{y},1/4 [0,v,0] \\
& & & 1/2,\bar{y},3/4 [0,v,0] \\
& & & 1/2,y,3/4 [0,v,0] \\
8 & k & .2' & 0,y,1/4 [u,0,w] \\
& & & 0,\bar{y},1/4 [u,0,\bar{w}] \\
& & & 0,\bar{y},3/4 [u,0,\bar{w}] \\
& & & 0,y,3/4 [u,0,w] \\
8 & j & .2' & x,1/2,1/4 [0,v,w] \\
& & & \bar{x},1/2,1/4 [\bar{u},\bar{v},0] \\
& & & \bar{x},1/2,3/4 [\bar{u},\bar{v},0] \\
& & & x,1/2,3/4 [0,v,w] \\
8 & i & .2' & x,0,1/4 [0,v,w] \\
& & & \bar{x},0,1/4 [\bar{u},\bar{v},0] \\
& & & \bar{x},0,3/4 [\bar{u},\bar{v},0] \\
& & & x,0,3/4 [0,v,w] \\
4 & h & 2'2' & 1/2,1/2,1/4 [0,v,0] \\
& & & 1/2,1/2,3/4 [0,v,0] \\
4 & g & 2'2' & 0,1/2,1/4 [0,0,w] \\
& & & 0,1/2,3/4 [0,0,\bar{w}] \\
4 & f & 2'2' & 1/2,0,1/4 [0,v,0] \\
& & & 1/2,0,3/4 [0,v,0] \\
4 & e & 2'2' & 0,0,1/4 [0,0,w] \\
& & & 0,0,3/4 [0,0,\bar{w}] \\
4 & d & .2'm' & 1/2,0,0 [u,v,0] \\
& & & 1/2,0,1/2 [\bar{u},\bar{v},0] \\
4 & c & .2'm' & 0,1/2,0 [0,0,0] \\
& & & 0,1/2,1/2 [0,0,0] \\
4 & b & .2'm' & 1/2,1/2,0 [u,v,0] \\
& & & 1/2,1/2,1/2 [\bar{u},\bar{v},0] \\
4 & a & .2'm' & 0,0,0 [0,0,0] \\
& & & 0,0,1/2 [0,0,0] \\
\end{array}
\]

**Symmetry of Special Projections**

Along [0,0,1]  \( p_{2a} \) 2mm  
Along [1,0,0]  \( p2mm1' \)  
Along [0,1,0]  \( p_c \) 2mm

\( a^* = a \quad b^* = b \)

Origin at 0,0,z

Origin at x,0,0

Origin at 1/2,y,0
### Symmetry Operations

**For (0,0,0) + set**

1. $1$
   - $(1|0,0,0)$
2. $2$
   - $0,0,z$
   - $(2|0,0,0)$
3. $2'$
   - $0,y,1/4$
   - $(2|0,0,1/2)'$
4. $2'$
   - $x,0,1/4$
   - $(2|0,0,1/2)'$

**For (1,0,0)' + set**

1. $t'(1,0,0)$
   - $(1|1,0,0)'$
2. $2'$
   - $1/2,0,z$
   - $(2|1,0,0)'$
3. $2$
   - $1/2,y,1/4$
   - $(2|1,0,1/2)$
4. $2$(1,0,0)
   - $x,0,1/4$
   - $(2|1,0,1/2)$

### Origin

At center (2/m) at c'c'2/m

### Asymmetric unit

$0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$
Generators selected  (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1,0,0)' +</td>
</tr>
<tr>
<td>8 q ..m</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 p ..2'</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 o ..2</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 n ..2'</td>
<td>1/2,1/2,z [u,v,0]</td>
<td>1/2,1/2,z [u,v,0]</td>
<td>1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>8 m ..2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 l ..2</td>
<td>1/2,y,1/4 [0,v,0]</td>
<td>1/2,y,1/4 [0,v,0]</td>
<td>1/2,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 k ..2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 j ..2'</td>
<td>x,1/2,1/4 [0,v,w]</td>
<td>x,1/2,1/4 [0,v,w]</td>
<td>x,1/2,1/4 [0,v,w]</td>
</tr>
<tr>
<td>8 i ..2'</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>4 h 2'2'</td>
<td>1/2,1/2,1/4 [0,v,0]</td>
<td>1/2,1/2,1/4 [0,v,0]</td>
<td>1/2,1/2,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 g 2'2</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 f 2'2'</td>
<td>1/2,0,1/4 [0,v,0]</td>
<td>1/2,0,1/4 [0,v,0]</td>
<td>1/2,0,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 e 2'2'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 d ..2'm</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c ..2/m</td>
<td>0,1/2,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 b ..2'm</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a ..2/m</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2mm1'  
  - a* = a  b* = b  
  - Origin at 0,0,z
- Along [1,0,0] p2mm1'  
  - a* = b  b* = c/2  
  - Origin at x,0,0
- Along [0,1,0] p2v, 2mm  
  - a* = -a  b* = c/2  
  - Origin at 0,y,0
**Symmetry Operations**

For \((0,0,0) + \text{ set}\):

1. \((1,0,0)\)
2. \((2',1/2,0,z)\)
3. \((3,1/2,y,1/4)\)
4. \((4,2,0,1/4)\)
5. \((5,0,1/2)\)
6. \((6,1,0,0)\)
7. \((7,1,0,1/2)\)
8. \((8,0,1/2)\)

For \((1,0,0)' + \text{ set}\):

1. \((1,0,0)'\)
2. \((2,1,0,0)'\)
3. \((3,1,0,0)'\)
4. \((4,2,1,0,0)'\)
5. \((5,0,0,0)'\)
6. \((6,0,0,0)'\)
7. \((7,0,0,0)'\)
8. \((8,0,0,0)'\)
Generators selected  (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 q .m'</td>
<td>x,y,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 p .2'</td>
<td>1/2,0,z [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 o .2</td>
<td>0,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 n .2'</td>
<td>1/2,1/2,z [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 m .2</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 l .2'</td>
<td>1/2,y,1/4 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 k .2</td>
<td>0,y,1/4 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 j .2</td>
<td>x,1/2,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 i .2</td>
<td>x,0,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 h 22'2'</td>
<td>1/2,1/2,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 g 222</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 f 22'2'</td>
<td>1/2,0,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e 222</td>
<td>0,0,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 d .2'm'</td>
<td>1/2,0,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 c .2'm'</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b .2'm'</td>
<td>1/2,1/2,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 a .2'm'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1]  $p_{2\alpha} 2m'm'$  
- Along [1,0,0]  $p2mm1'$  
- Along [0,1,0]  $p_{2\alpha} 2m'm'$  

Origin at 0,0,z

$\mathbf{a}^* = \mathbf{a}$  $\mathbf{b}^* = \mathbf{b}$

Origin at $x,0,0$

$\mathbf{a}^* = -\mathbf{a}$  $\mathbf{b}^* = c/2$

Origin at 0,0,0
Origin at center (2/m') at cc2/m'

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

1. $T' (1|0,0,0)$
2. $T' (1|0,0,0')$
3. $T' (1|2,0,0)$

For (1,0,0) + set

1. $T' (0,1,0)$
2. $T' (0,1,0)$
3. $T' (0,1,0)$

4. $1 (0,0,0)$
5. $2 (0,0,0)$
6. $2 (0,0,0)$

7. $2 (0,0,0)$
8. $2 (0,0,0)$
9. $2 (0,0,0)$

10. $2 (0,0,0)$
11. $2 (0,0,0)$
12. $2 (0,0,0)$

13. $2 (0,0,0)$
14. $2 (0,0,0)$
15. $2 (0,0,0)$

16. $2 (0,0,0)$
17. $2 (0,0,0)$
18. $2 (0,0,0)$

19. $2 (0,0,0)$
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46. $2 (0,0,0)$
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50. $2 (0,0,0)$
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66. $2 (0,0,0)$

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68. $2 (0,0,0)$
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81. $2 (0,0,0)$

82. $2 (0,0,0)$
83. $2 (0,0,0)$
84. $2 (0,0,0)$

85. $2 (0,0,0)$
86. $2 (0,0,0)$
87. $2 (0,0,0)$

88. $2 (0,0,0)$
89. $2 (0,0,0)$
90. $2 (0,0,0)
Continued

Generators selected
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 r..m'</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 q..m'</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 p..2'</td>
<td>1/2,0,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 o..2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>8 n..2</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 m..2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 l..2</td>
<td>1/2,y,1/4 [0,v,0]</td>
<td>1/2,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 k..2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 j..2</td>
<td>x,1/2,1/4 [u,0,0]</td>
<td>x,1/2,1/4 [u,0,0]</td>
</tr>
<tr>
<td>8 i..2'</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>4 h 222</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 g 22' 2'</td>
<td>0,1/2,1/4 [u,0,0]</td>
<td>0,1/2,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 f 2' 2'</td>
<td>1/2,0,1/4 [0,v,0]</td>
<td>1/2,0,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 e 2' 2'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 d ..2'/m'</td>
<td>1/2,0,0 [u,v,0]</td>
<td>1/2,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 c ..2'/m'</td>
<td>0,1/2,0 [u,v,0]</td>
<td>0,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b ..2'/m'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a ..2'/m'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_c 2mm

a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2mm1'

a* = b  b* = c/2
Origin at x,0,0

Along [0,1,0] p2mm1'

a* = c/2  b* = a
Origin at 0,y,0
Origin: at 222/n, at 1/4,1/4,0 from \( \bar{1} \)

Asymmetric unit: 

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations:

\begin{align*}
(1) \ \bar{1} & \quad (1) \ 0,0,0 \\
(2) \ \bar{2} & \quad (2) \ 0,0,z & (3) \ \bar{2} & \quad (3) \ 0,y,0 & (4) \ \bar{2} & \quad (4) \ x,0,0 \\
(5) \ \bar{1} & \quad (5) \ 1/4,1/4,0 & (6) \ n & \quad (6) \ (1/2,1/2,0) \ x,y,0 & (7) \ a & \quad (7) \ (1/2,0,0) \ x,1/4,z & (8) \ b & \quad (8) \ (0,1/2,0) \ 1/4,y,z \\
(1) & \quad (1) \ \bar{1}/2,1/2,0 & (2) & \quad (2) z \ \bar{1}/2,1/2,0 & (3) & \quad (3) y \ \bar{1}/2,1/2,0 & (4) & \quad (4) x \ \bar{1}/2,1/2,0 & (5) & \quad (5) \ \bar{1}/2,1/2,0
\end{align*}
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>8 m 1</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(1) x, y, z [u, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [u, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) x, y, z [u, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) x, y, z [u, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) x + 1/2, y + 1/2, z [u, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(6) x + 1/2, y + 1/2, z [u, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) x + 1/2, y + 1/2, z [u, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(8) x + 1/2, y + 1/2, z [u, v, w]</td>
<td></td>
</tr>
</tbody>
</table>

4 l .2 0, 1/2, z [0, 0, w] 0, 1/2, z [0, 0, w] 1/2, 0, z [0, 0, w] 1/2, 0, z [0, 0, w]
4 k .2 0, 0, z [0, 0, w] 0, 0, z [0, 0, w] 1/2, 1/2, z [0, 0, w] 1/2, 1/2, z [0, 0, w]
4 j .2 0, y, 1/2 [0, v, 0] 0, y, 1/2 [0, v, 0] 1/2, y + 1/2, 1/2 [0, v, 0] 1/2, y + 1/2, 1/2 [0, v, 0]
4 i .2 0, y, 0 [0, v, 0] 0, y, 0 [0, v, 0] 1/2, y + 1/2, 0 [0, v, 0] 1/2, y + 1/2, 0 [0, v, 0]
4 h 2.. x, 0, 1/2 [u, 0, 0] x, 0, 1/2 [u, 0, 0] x + 1/2, 1/2, 1/2 [u, 0, 0] x + 1/2, 1/2, 1/2 [u, 0, 0]
4 g 2.. x, 0, 0 [u, 0, 0] x, 0, 0 [u, 0, 0] x + 1/2, 1/2, 0 [u, 0, 0] x + 1/2, 1/2, 0 [u, 0, 0]
4 f 1.. 1/4, 1/4, 1/2 [u, v, w] 3/4, 3/4, 1/2 [u, v, w] 3/4, 1/4, 1/2 [u, v, w] 1/4, 3/4, 1/2 [u, v, w]
4 e 1.. 1/4, 1/4, 0 [u, v, w] 3/4, 3/4, 0 [u, v, w] 3/4, 1/4, 0 [u, v, w] 1/4, 3/4, 0 [u, v, w]
2 d 222 0, 0, 1/2 [0, 0, 0] 1/2, 1/2, 1/2 [0, 0, 0]
2 c 222 1/2, 0, 1/2 [0, 0, 0] 1/2, 1/2 [0, 0, 0]
2 b 222 1/2, 0, 0 [0, 0, 0] 0, 1/2, 0 [0, 0, 0]
2 a 222 0, 0, 0 [0, 0, 0] 1/2, 1/2, 0 [0, 0, 0]

Symmetry of Special Projections

Along [0, 0, 1] c_p, 2m' m'  
Along [1, 0, 0] p_{2a}, 2m' m'  
Along [0, 1, 0] p_{2a}, 2m' m'

a^* = a  b^* = b  
a^* = b/2  b^* = c  
a^* = -a/2  b^* = c

Origin at 0, 0, z  
Origin at x, 0, 0  
Origin at 0, y, 0
Orthorhombic

50.2.378

Pban1’

mmm1’

1’

Origin at 222/n1’, at 1/4,1/4,0 from 1’

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For 1 + set

(1) 1
(1|0,0,0)

(5) 1’/4,1/4,0
(1|2,1/2,0)

(2) 2 0,0,z
(2|0,0,0)

(6) n (1/2,1/2,0) x,y,0
(mz|1/2,1/2,0)

(3) 2 0,y,0
(2|0,0,0)

(7) a (1/2,0,0) x,1/4,z
(my|1/2,1/2,0)

(4) 2 x,0,0
(2z|0,0,0)

For 1’ + set

(1) 1’
(1|0,0,0)’

(5) 1’/4,1/4,0
(1|2,1/2,0)’

(2) 2’ 0,0,z
(2z|0,0,0)’

(6) n’ (1/2,1/2,0) x,y,0
(mz|1/2,1/2,0)’

(3) 2’ 0,y,0
(2|0,0,0)’

(7) a’ (1/2,0,0) x,1/4,z
(my|1/2,1/2,0)’

(4) 2’ x,0,0
(2z|0,0,0)’

(8) b’ (0,1/2,0) 1/4,y,z
(mz|1/2,1/2,0)’
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 m 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [0,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = c</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin: at 22'2'/n, at 1/4,1/4,0 from \( \bar{1} \)

Asymmetric unit: \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations:

1. \( \bar{1} \)
   - \( 1 \ | \ 0,0,0 \)
   - \( \bar{1} \ | \ 1/2,1/2,0 \)

2. \( 2' \)
   - \( 0,0,z \ | \ 0,0,0' \)
   - \( 0,y,0 \ | \ 0,0,0' \)
   - \( x,0,0 \ | \ 0,0,0 \)

3. \( \bar{1}' \)
   - \( 1/4,1/4,0 \ | \ 1/4,1/4,0' \)
   - \( x,y,0 \ | \ 1/2,1/2,0 \)
   - \( 1/4,z \ | \ 1/2,1/2,0 \)
   - \( 1/4,y,z \ | \ 1/2,1/2,0 \)

4. \( a \)
   - \( 1/2,0,0 \ | \ 0,0,0 \)
   - \( 1/2,1/2,0 \ | \ 1/2,1/2,0 \)

5. \( b' \)
   - \( 0,1/2,0 \ | \ 1/4,0,0' \)
   - \( 1/2,1/2,0 \ | \ 1/2,1/2,0' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 m 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w] (6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z [u,v,w] (8) x+1/2,y+1/2,z [u,v,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c_p, 2mm'</th>
<th>Along [1,0,0]</th>
<th>p 2mm</th>
<th>Along [0,1,0]</th>
<th>p_{2a}, 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a, b* = b</td>
<td>a* = b/2, b* = c</td>
<td>a* = c, b* = a/2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,0
Origin at 2'2'2/n', at 1/4,1/4,0 from 1'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
    (1 | 0,0,0)

(2) 2  0,0,z
    (2_z | 0,0,0)

(3) 2' 0,y,0
    (2_y | 0,0,0')

(4) 2' x,0,0
    (2_x | 0,0,0')

(5) 1
    (1 | 1/2,1/2,0)

(6) n' (1/2,1/2,0) x,y,0
    (m_z | 1/2,1/2,0')

(7) a (1/2,0,0) x,1/4,z
    (m_y | 1/2,1/2,0)

(8) b (0,1/2,0) 1/4,y,z
    (m_z | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

8 m 1  (1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  
(3) x,y,z [u,v,w]  (4) x,y,z [u,v,w]  
(5) x+1/2,y+1/2,z [u,v,w]  (6) x+1/2,y+1/2,z [u,v,w]  
(7) x+1/2,y+1/2,z [u,v,w]  (8) x+1/2,y+1/2,z [u,v,w]  

Coordinates

4 l 0.1/2,z [0.0,w]  0.1/2,z [0.0,w]  1/2.0,z [0.0,w]  1/2.0,z [0.0,w]  
4 k 0.0,z [0.0,w]  0.0,z [0.0,w]  1/2.0,z [0.0,w]  1/2.0,z [0.0,w]  
4 j 0.0,1/2 [u,0,w]  0.0,1/2 [u,0,w]  1/2.0,1/2 [u,0,w]  1/2.0,1/2 [u,0,w]  
4 i 0.0,0 [u,0,w]  0.0,0 [u,0,w]  1/2.0,1/2 [u,0,w]  1/2.0,1/2 [u,0,w]  
4 h x,0,1/2 [0,v,w]  x,0,1/2 [0,v,w]  x+1/2,1/2,1/2 [0,v,w]  x+1/2,1/2,1/2 [0,v,w]  
4 g x,0,0 [0,v,w]  x,0,0 [0,v,w]  x+1/2,1/2,2 [0,v,w]  x+1/2,1/2,2 [0,v,w]  
4 f 1/4,1/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]  
4 e 1/4,1/4,0 [0,0,0]  3/4,3/4,0 [0,0,0]  3/4,3/4,0 [0,0,0]  1/4,3/4,0 [0,0,0]  
2 d 0.0,1/2 [0,0,w]  1/2.1,2.1,2 [0,0,w]  
2 c 1/2.0,1/2 [0,0,w]  0.1,2.1,2 [0,0,w]  
2 b 1/2.0,0 [0,0,w]  0.1,2.0 [0,0,w]  
2 a 0.0,0 [0,0,w]  1/2.1,2.0 [0,0,w]  

Symmetry of Special Projections

Along [0,0,1]   c2mm  
Along [1,0,0]   p2a-2mm  
Along [0,1,0]   p2a-2mm  

\[ a^* = a \quad b^* = b \]  
Origin at 0,0,z  

\[ a^* = b/2 \quad b^* = c \]  
Origin at x,1/4,0  

\[ a^* = -a/2 \quad b^* = c \]  
Origin at 1/4,y,0
Pb'a'n  
50.5.381  
Origin  at 2'2'2/n, at 1/4,1/4,0 from $\bar{1}$

Asymmetric unit  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1  
(1 0,0,0)

(2) 2 0,0,z  
(2 0,0,0)

(3) $2'$ 0,y,0  
(2,0,0,0)'

(4) $2'$ x,0,0  
(2,0,0,0)'

(5) $\bar{1}$ 1/4,1/4,0  
($\bar{1}$ 1/2,1/2,0)

(6) n (1/2,1/2,0) x,y,0  
(m_z 1/2,1/2,0)

(7) a' (1/2,0,0) x,1/4,z  
(m_y 1/2,1/2,0)'

(8) b' (0,1/2,0) 1/4,y,z  
(m_x 1/2,1/2,0)'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>8</th>
<th>m</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) ( \bar{x}, \bar{y}, z ) [( \bar{u}, \bar{v}, w )]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) ( \bar{x}, y, z ) [( u, \bar{v}, w )]</td>
<td>(4) x,y,( \bar{z} ) [u,v,w]</td>
</tr>
<tr>
<td></td>
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<td></td>
<td>(5) x+1/2, ( \bar{y} ), 1/2, z [u,v,w]</td>
<td>(6) x+1/2, y+1/2, ( \bar{z} ) [u,( \bar{v}, w )]</td>
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<tr>
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<td></td>
<td>(7) x+1/2, ( \bar{y} ), 1/2, z [u,( \bar{v}, w )]</td>
<td>(8) x+1/2, y+1/2, ( \bar{z} ) [u,( \bar{v}, w )]</td>
</tr>
</tbody>
</table>

4 l  .2  0,1/2, z [0,0,w]  0,1/2, z [0,0,w]  1/2,0, z [0,0,w]  1/2,0, z [0,0,w]
4 k  .2  0,0, z [0,0,w]  0,0, z [0,0,w]  1/2,1/2, z [0,0,w]  1/2,1/2, z [0,0,w]
4 j  .2'  0,y,1/2 [u,0,w]  0,\( \bar{y} \), 1/2 [u,0,w]  1/2,\( \bar{y} \), 1/2,1/2 [u,0,w]  1/2,\( \bar{y} \), 1/2,1/2 [u,0,w]
4 i  .2'  0,y,0 [u,0,w]  0,\( \bar{y} \), 0 [u,0,w]  1/2,\( \bar{y} \), 1/2,0 [u,0,w]  1/2,\( \bar{y} \), 1/2,0 [u,0,w]
4 h  2'.. x,0,1/2 [0,v,w]  \( \bar{x} \), 0,1/2 [0,\( \bar{v}, w \)]  \( \bar{x} \), +1/2,1/2,1/2 [0,\( \bar{v}, w \)]  \( \bar{x} \), +1/2,1/2,1/2 [0,\( \bar{v}, w \)]
4 g  2'.. x,0,0 [0,v,w]  \( \bar{x} \), 0,0 [0,\( \bar{v}, w \)]  \( \bar{x} \), +1/2,1/2,0 [0,\( \bar{v}, w \)]  \( \bar{x} \), +1/2,1/2,0 [0,\( \bar{v}, w \)]
4 f  1/4,1/4,1/2 [u,v,w]  3/4,3/4,1/2 [u,\( \bar{v}, w \)]  3/4,1/4,1/2 [u,\( \bar{v}, w \)]  1/4,3/4,1/2 [u,v,w]
4 e  1/4,1/4,0 [u,v,w]  3/4,3/4,0 [u,\( \bar{v}, w \)]  3/4,1/4,0 [u,\( \bar{v}, w \)]  1/4,3/4,0 [u,v,w]
2 d  2'2'  0,0,1/2 [0,0,w]  1/2,1/2,1/2 [0,0,w]
2 c  2'2'  1/2,0,1/2 [0,0,w]  0,1/2,1/2 [0,0,w]
2 b  2'2'  1/2,0,0 [0,0,w]  0,1/2,0 [0,0,w]
2 a  2'2'  0,0,0 [0,0,w]  1/2,1/2,0 [0,0,w]

Symmetry of Special Projections

- Along [0,0,1]  \( c_p \), 2mm
- Along [1,0,0]  p2'mm'
- Along [0,1,0]  p2'mm'

\( a^* = a \)  \( b^* = b \)  \( a^* = -c \)  \( b^* = -b/2 \)  \( a^* = c \)  \( b^* = a/2 \)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
**Origin**  at 2'22'/n', at 1/4,1/4,0 from $\bar{1}$

**Asymmetric unit**  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Matrix</th>
<th>Site</th>
<th>Site'</th>
<th>Site''</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>$1$</td>
<td>0,0,0</td>
<td>0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>2</td>
<td>2'</td>
<td>$2' \ 0,0,z$</td>
<td>$(2_2,0,0,0)'$</td>
<td>0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>2</td>
<td>0,y,0</td>
<td>0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>4</td>
<td>2'</td>
<td>$2' x,0,0$</td>
<td>$(2_2,0,0,0)'$</td>
<td>0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>5</td>
<td>$\bar{1}$</td>
<td>$1/4,1/4,0$</td>
<td>$(\bar{1} \ 1/2,1/2,0)$</td>
<td>0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>6</td>
<td>n'</td>
<td>$n' (1/2,1/2,0)$</td>
<td>$(m_2,1/2,1/2,0)'$</td>
<td>1/4,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>7</td>
<td>a</td>
<td>$a (1/2,0,0)$</td>
<td>$(m_2,1/2,1/2,0)$</td>
<td>1/4,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>8</td>
<td>b'</td>
<td>$b' (0,1/2,0)$</td>
<td>$(m_2,1/2,1/2,0)'$</td>
<td>1/4,0</td>
<td>0,0,0</td>
</tr>
</tbody>
</table>
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) x+1/2, y+1/2, z [u,v,w]</td>
<td>(6) x+1/2, y+1/2, z [u,v,w]</td>
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<tr>
<td></td>
<td>(7) x+1/2, y+1/2, z [u,v,w]</td>
<td>(8) x+1/2, y+1/2, z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 l .2'</td>
<td>0,1/2,z [u,v,0] 0,1/2,z [u,v,0] 1/2,0,z [u,v,0] 1/2,0,z [u,v,0]</td>
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<tr>
<td>4 k .2'</td>
<td>0,0,z [u,v,0] 0,0,z [u,v,0] 1/2,1/2,z [u,v,0] 1/2,1/2,z [u,v,0]</td>
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</tr>
<tr>
<td>4 j .2</td>
<td>0,y,1/2 [0,v,0] 0,y,1/2 [0,v,0] 1/2,y+1/2,1/2 [0,v,0] 1/2,y+1/2,1/2 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 i .2</td>
<td>0,y,0 [0,v,0] 0,y,0 [0,v,0] 1/2,y+1/2,0 [0,v,0] 1/2,y+1/2,0 [0,v,0]</td>
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<td></td>
</tr>
<tr>
<td>4 h .2</td>
<td>x,0,1/2 [0,v,w] x,0,1/2 [0,v,w] x+1/2,1/2,1/2 [0,v,w] x+1/2,1/2,1/2 [0,v,w]</td>
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</tr>
<tr>
<td>4 g .2</td>
<td>x,0,0 [0,v,w] x,0,0 [0,v,w] x+1/2,1/2,0 [0,v,w] x+1/2,1/2,0 [0,v,w]</td>
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<td></td>
</tr>
<tr>
<td>4 f .1</td>
<td>1/4,1/4,1/2 [u,v,w] 3/4,3/4,1/2 [u,v,w] 3/4,1,4,1/2 [u,v,w] 1/4,3/4,1/2 [u,v,w]</td>
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</tr>
<tr>
<td>4 e .1</td>
<td>1/4,1/4,0 [u,v,w] 3/4,3/4,0 [u,v,w] 3/4,1/4,0 [u,v,w] 1/4,3/4,0 [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 d 2'2'</td>
<td>0,0,1/2 [0,v,0] 1/2,1,2,1/2 [0,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c 2'2'</td>
<td>1/2,0,1/2 [0,v,0] 1/2,1,2,1/2 [0,v,0]</td>
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<td></td>
</tr>
<tr>
<td>2 b 2'2'</td>
<td>1/2,0,0 [0,v,0] 0,1,2,0 [0,v,0]</td>
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<td></td>
</tr>
<tr>
<td>2 a 2'2'</td>
<td>0,0,0 [0,v,0] 1/2,1,2,0 [0,v,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] c2'mm'  
Along [1,0,0] p2'mm'  
Along [0,1,0] p2a', 2mm

a* = -b  b* = a  
a* = b/2  b* = c  
a* = -a/2  b* = c  
Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at 222/n', at 1/4,1/4,0 from \( \overline{1} \)

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2
\]

Symmetry Operations

1. \( 1 \)
2. \( 2 \quad 0,0,z \)
3. \( 2 \quad 0,y,0 \)
4. \( 2 \quad x,0,0 \)
5. \( \overline{1} \quad 1/4,1/4,0 \)
6. \( \overline{1} \quad 1/2,1/2,0 \)
7. \( a' \quad 1/2,0,0 \quad x,1/4,z \)
8. \( b' \quad 0,1/2,0 \quad 1/4,y,z \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 l .2</td>
<td>0,1/2,z [0,0,w]</td>
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<tr>
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<td>0,1/2,z [0,0,w]</td>
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<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
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<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
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<tr>
<td>4 k .2</td>
<td>0,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td></td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 j .2</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
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<td>0,y,1/2 [0,v,0]</td>
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<tr>
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<td>1/2,y+1/2,1/2 [0,v,0]</td>
</tr>
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<td>1/2,y+1/2,1/2 [0,v,0]</td>
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<tr>
<td>4 i .2</td>
<td>0,y,0 [0,v,0]</td>
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<td>0,y,0 [0,v,0]</td>
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<tr>
<td>4 h 2..</td>
<td>x,0,1/2 [u,0,0]</td>
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<td>2 b 222</td>
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<td>2 a 222</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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</tbody>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>c2m'm'</th>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
<th>Along [0,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = c</td>
<td>b* = a/2</td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z | Origin at x,0,0 | Origin at 0,y,0
**Origin** at 222/n, at 1/4,1/4,0 from \( \overline{1} \)

**Asymmetric unit**
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2|0,0,0)

(3) 2 0,y,0
(2|0,0,0)

(4) 2 x,0,0
(2|0,0,0)

(5) \( \overline{1} \) 1/4,1/4,0
(\( \overline{1} \)|1/2,1/2,0)

(6) n (1/2,1/2,0) x,y,0
(m\( _{z} \)|1/2,1/2,0)

(7) a (1/2,0,0) x,1/4,z
(m\( _{y} \)|1/2,1/2,0)

(8) b (0,1/2,0) 1/4,y,z
(m\( _{x} \)|1/2,1/2,0)

For (0,0,1)’ + set

(1) t’ (0,0,1)
(1|0,0,1)’

(2) 2’ (0,0,1) 0,0,z
(2|0,0,1)’

(3) 2’ 0,y,1/2
(2|0,0,1)’

(4) 2’ x,0,1/2
(2|0,0,1)’

(5) \( \overline{1} \)’ 1/4,1/4,1/2
(\( \overline{1} \)|1/2,1/2,1)’

(6) n’ (1/2,1/2,0) x,y,1/2
(m\( _{z} \)|1/2,1/2,1)’

(7) n’ (1/2,0,1) x,1/4,z
(m\( _{y} \)|1/2,1/2,1)’

(8) n’ (0,1/2,1) 1/4,y,z
(m\( _{x} \)|1/2,1/2,1)’
Generators selected: (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 m 1</td>
<td>(0,0,0) + (0,0,1)′ +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<td>(3) x,y,z [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
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<tr>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>(6) x+y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(7) x+1/2,y+1/2,z [u,v,w]</td>
<td>(8) x+y+1/2,z [u,v,w]</td>
</tr>
</tbody>
</table>

### Coordinates

| l | 0.1/2,z [0,0,w] | 0.1/2,z [0,0,w] | 0.1/2,z [0,0,w] | 1/2,0,z [0,0,w] |
| k | 0.0,z [0,0,w]   | 0.0,z [0,0,w]   | 1/2,1/2,z [0,0,w] | 1/2,1/2,z [0,0,w] |
| j | 0.0,y,1/2 [u,0,w] | 0.0,y,1/2 [u,0,w] | 1/2,0,y+1/2,1/2 [u,0,w] | 1/2,0,y+1/2,1/2 [u,0,w] |
| i | 0.0,y,0 [0,v,0]  | 0.0,y,0 [0,v,0]  | 1/2,0,y+1/2,0 [0,v,0] | 1/2,0,y+1/2,0 [0,v,0] |
| h | x,0,1/2 [0,v,w]  | x,0,1/2 [0,v,w]  | x+1/2,1/2,1/2 [0,v,w] | x+1/2,1/2,1/2 [0,v,w] |
| g | x,0,0 [u,0,0]    | x,0,0 [u,0,0]    | x+1/2,1/2,0 [u,0,0] | x+1/2,1/2,0 [u,0,0] |
| f | 1/4,1/4,1/2 [0,0,0] | 3/4,3/4,1/2 [0,0,0] | 3/4,1/4,1/2 [0,0,0] | 1/4,3/4,1/2 [0,0,0] |
| e | 1/4,1/4,0 [u,v,w] | 3/4,3/4,0 [u,v,w] | 3/4,1/4,0 [u,v,w] | 1/4,3/4,0 [u,v,w] |
| d | 0.0,1/2 [0,0,w]  | 1/2,1/2,1/2 [0,0,w] | 1/2,1/2,1/2 [0,0,w] | 1/2,1/2,1/2 [0,0,w] |
| c | 1/2,0,1/2 [0,0,w] | 1/2,0,1/2 [0,0,w] | 1/2,0,1/2 [0,0,w] | 1/2,0,1/2 [0,0,w] |
| b | 1/2,0,0 [0,0,0]  | 1/2,0,0 [0,0,0]  | 1/2,0,0 [0,0,0] | 1/2,0,0 [0,0,0] |
| a | 0.0,0 [0,0,0]    | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |

### Symmetry of Special Projections

Along [0,0,1] c2mm1′
Along [1,0,0] p2c 2mm
Along [0,1,0] p2c 2mm

\[
a^* = a \quad b^* = b
\]
Origin at 0,0,z

\[
a^* = b/2 \quad b^* = c
\]
Origin at x,1/4,1/2

\[
a^* = c \quad b^* = a/2
\]
Origin at 1/4,y,1/2
Origin at 222/n, at 1/4,1/4,0 from T

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. T (1|0,0,0)

2. T' 0,0,z (2|0,0,0)'

3. T' 0,y,0 (2|0,0,0)'

4. T' x,0,0 (2|0,0,0)'

5. T 1/4,1/4,0 (1|1/2,1/2,0)'

6. n (1/2,1/2,0) x,y,0 (m|1/2,1/2,0)

7. a (1/2,0,0) x,1/4,z (m|1/2,1/2,0)

8. b' (0,1/2,0) 1/4,y,z (m|1/2,1/2,0)'

For (0,0,1) + set

1. T' (0,0,1) (1|0,0,1)'

2. T 0,0,1 (2|0,0,1)'

3. T 0,y,1/2 (2|0,0,1)'

4. T' x,0,1/2 (2|0,0,1)'

5. T 1/4,1/4,1/2 (1|1/2,1/2,1)'

6. n' (1/2,1/2,0) x,y,1/2 (m|1/2,1/2,1)'

7. n' (1/2,0,1) x,1/4,z (m|1/2,1/2,1)'

8. n (0,1/2,1) 1/4,y,z (m|1/2,1/2,1)'
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
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<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
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<td></td>
<td>(4) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>8 l .2'</td>
<td>0,1/2,z [u,v,0] 0,1/2,z [u,v,0] 1/2,0,z [u,v,0] 1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 k .2'</td>
<td>0,0,z [u,v,0] 0,0,z [u,v,0] 1/2,1/2,z [u,v,0] 1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>8 j .2.</td>
<td>0,y,1/2 [0,v,0] 0,y,1/2 [0,v,0] 1/2,y+1/2,1/2 [0,v,0] 1/2,y+1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 i .2'.</td>
<td>0,y,0 [u,0,w] 0,y,0 [u,0,w] 1/2,y+1/2,0 [u,0,w] 1/2,y+1/2,0 [u,0,w]</td>
</tr>
<tr>
<td>8 h 2'.</td>
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<tr>
<td>8 g 2..</td>
<td>x,0,0 [u,0,0] x,0,0 [u,0,0] x+1/2,1/2,0 [u,0,0] x+1/2,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>8 f 1 1/4,1/4,1/2 [u,v,w] 3/4,3/4,1/2 [u,v,w] 3/4,3/4,1/2 [u,v,w] 1/4,3/4,1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 e 1 1/4,1/4,0 [0,0,0] 3/4,3/4,0 [0,0,0] 3/4,1/4,0 [0,0,0] 1/4,3/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 d 2'2'</td>
<td>0,0,1/2 [0,v,0] 1/2,1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 c 2'2'</td>
<td>1/2,0,1/2 [0,v,0] 1/2,1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 b 22'</td>
<td>1/2,0,0 [u,0,0] 0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 a 22'</td>
<td>0,0,0 [u,0,0] 1/2,1/2,0 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1' 
Along [1,0,0] p2a-2mm 
Along [0,1,0] p_c-2mm 
\( a^* = a \) \( b^* = b \) 
\( a^* = -c \) \( b^* = b/2 \) 
\( a^* = c \) \( b^* = a/2 \) 
Origin at 0,0,z 
Origin at x,0,0 
Origin at 0,y,1/2
Origin at \(2'2'2'/n\), at \(1/4,1/4,0\) from \(\overline{1}\)

Asymmetric unit \(0 < x < 1/2;\) \(0 < y < 1/2;\) \(0 < z < 1/2\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \quad (1|0,0,0)\)
2. \(2 \quad 0,0,z\) \((2_z|0,0,0)\)
3. \(2' \quad 0,y,0\) \((2_y|0,0,0)'\)
4. \(2' \quad x,0,0\) \((2_x|0,0,0)'\)
5. \(\overline{1} \quad 1/4,1/4,0\) \((\overline{1}|1/2,1/2,0)\)
6. \(n \quad (1/2,1/2,0) \quad x,y,0\) \((m_z|1/2,1/2,0)\)
7. \(a' \quad (1/2,0,0) \quad x,1/4,z\) \((m_y|1/2,1/2,0)'\)
8. \(b' \quad (0,1/2,0) \quad 1/4,y,z\) \((m_x|1/2,1/2,0)'\)

For \((0,0,1)' + \) set

1. \(t' \quad (0,0,1)\)
2. \(2' \quad (0,0,1) \quad 0,0,z\) \((2_z|0,0,1)'\)
3. \(2 \quad 0,y,1/2\) \((2_y|0,0,1)\)
4. \(2 \quad x,0,1/2\) \((2_x|0,0,1)\)
5. \(\overline{1} \quad 1/4,1/4,1/2\) \((\overline{1}|1/2,1/2,1)\)
6. \(n' \quad (1/2,1/2,0) \quad x,y,1/2\) \((m_z|1/2,1/2,1)'\)
7. \(n \quad (1/2,0,1) \quad x,1/4,z\) \((m_y|1/2,1/2,1)'\)
8. \(n \quad (0,1/2,1) \quad 1/4,y,z\) \((m_x|1/2,1/2,1)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

<table>
<thead>
<tr>
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<th>Coordinates</th>
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<td>(0,0,0) + (0,0,1) +</td>
</tr>
<tr>
<td>8 l</td>
<td>0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z [0,0,w]</td>
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</tr>
<tr>
<td>8 j</td>
<td>0,1/2 [0,v,0] 0,1/2 [0,v,0] 1/2,1/2 [0,v,0] 1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>0,0,0 [u,0,w] 0,0,0 [u,0,w] 1/2,0 [u,0,w] 1/2,0 [u,0,w]</td>
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<tr>
<td>8 h</td>
<td>x,0,1/2 [u,0,0] x,0,1/2 [u,0,0] x+1/2,1/2 [u,0,0] x+1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>x,0,0 [u,0,0] x,0,0 [u,0,0] x+1/2,1/2 [u,0,0] x+1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 f</td>
<td>1/4,1/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 1/4,3/4,1/2 [0,0,0]</td>
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<tr>
<td>8 e</td>
<td>1/4,1/4,1/2 [u,v,w] 3/4,3/4,1/2 [u,v,w] 3/4,3/4,1/2 [u,v,w] 1/4,3/4,1/2 [u,v,w]</td>
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<td>4 d</td>
<td>0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>4 c</td>
<td>1/2,0,1/2 [0,0,0] 0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>1/2,0,0 [0,0,w] 0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,0,w] 1/2,1/2,0 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1]: c2mm1'
- Along [1,0,0]: p2a, 2m1m'
- Along [0,1,0]: p2a, 2m1m'

\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \quad \mathbf{c}^* = \mathbf{c} \) 

Origin at 0,0,1/2

\( \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \) 

Origin at x,0,1/2

\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a}/2 \) 

Origin at 0,y,0
Origin: at center (2/m) at 2,2/ma

Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations:

1. 1 (1 0 0 0)
2. 2 1/4,0,z (2 1/2,0,0)
3. 2 0,y,0 (2 0,0,0)
4. 2 (1/2,0,0) x,0,0 (2,1/2,0,0)
5. 1 (1 0 0 0)
6. a (1/2,0,0) x,y,0 (m 1/2,0,0)
7. m x,0,z (m 0,0,0)
8. m 1/4,y,z (m 1/2,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(2) x+1/2,y,z [u,v,w]</td>
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<td>(3) x,y,z [u,v,w]</td>
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<td>(4) x+1/2,y,z [u,v,w]</td>
</tr>
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<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(6) x+1/2,y,z [u,v,w]</td>
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<td>(7) x,y,z [u,v,w]</td>
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<td>(8) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 k m..</td>
<td>1/4,y,z [u,0,0]</td>
</tr>
<tr>
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<td>1/4,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,y,z [u,0,0]</td>
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<td>3/4,y,z [u,0,0]</td>
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<td>4 j .m.</td>
<td>x,1/2,z [0,v,0]</td>
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<td>x+1/2,1/2,z [0,v,0]</td>
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<td>x,1/2,z [0,v,0]</td>
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<td>x+1/2,1/2,z [0,v,0]</td>
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<td>x,0,z [0,v,0]</td>
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<td>2 d .2/m.</td>
<td>0,1/2,1/2 [0,v,0]</td>
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<td>1/2,0,0 [0,v,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p$_{2a}$ 2mm

| a* = a/2  b* = b |
| Origina at 1/4,0,z |

Along [1,0,0] p2mm1'  

| a* = b  b* = c |
| Origina at x,0,0 |

Along [0,1,0] p2mg1'  

| a* = -a  b* = c |
| Origina at 0,y,0 |
Origin at center (2/m1') at 2, 2/ma1'

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For 1 + set

(1) 1 (1) |0,0,0)
(2) 2 1/4,0,z (2z|1/2,0,0)
(3) 2 y,0 (2z|0,0,0)
(4) 2 (1/2,0,0) x,0,0 (2z|1/2,0,0)
(5) 1 (1) |0,0,0)
(6) a (1/2,0,0) x,y,0 (mz|1/2,0,0)
(7) m x,0,z (my|0,0,0)
(8) m 1/4,y,z (my|1/2,0,0)

For 1' + set

(1) 1' (1) |0,0,0')
(2) 2' 1/4,0,z (2z|1/2,0,0')
(3) 2' y,0 (2z|0,0,0')
(4) 2' (1/2,0,0) x,0,0 (2z|1/2,0,0')
(5) 1' (1) |0,0,0')
(6) a' (1/2,0,0) x,y,0 (mz|1/2,0,0')
(7) m' x,0,z (my|0,0,0')
(8) m' 1/4,y,z (my|1/2,0,0')
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

<table>
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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
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<tbody>
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<td>8 l 11' (1) x,y,z [0,0,0]</td>
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<tr>
<td>(2) $x+1/2,y,z$ [0,0,0]</td>
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<tr>
<td>(3) $x,y,z$ [0,0,0]</td>
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<td>(4) $x+1/2,y,z$ [0,0,0]</td>
</tr>
<tr>
<td>(5) $x,y,z$ [0,0,0]</td>
</tr>
<tr>
<td>4 k m..1' 1/4,y,z [0,0,0]</td>
</tr>
<tr>
<td>4 j .m.1' x,1/2,z [0,0,0]</td>
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<tr>
<td>4 i .m.1' x,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 h .2.1' 0,y,1/2 [0,0,0]</td>
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<td>4 g .2.1' 0,y,0 [0,0,0]</td>
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<tr>
<td>2 f mm21' 1/4,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 e mm21' 1/4,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d .2/m.1' 0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c .2/m.1' 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b .2/m.1' 0,1,2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a .2/m.1' 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p2mm1'</th>
<th>Along [1,0,0] p2mm1'</th>
<th>Along [0,1,0] p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = a/2$</td>
<td>$a^* = b$</td>
<td>$a^* = -a$</td>
</tr>
<tr>
<td>$b^* = b$</td>
<td>$b^* = c$</td>
<td>$b^* = c$</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Pm'\text{ma} 
\begin{align*}
51.3.389 & 
\end{align*}

m'\text{mm} 
\begin{align*}
P2_1/m'2'/m2'/a & 
\end{align*}

Orthorhombic

\begin{align*}
\text{Origin at center (}2'/\text{m}) \text{ at } 2,2'/\text{ma}
\end{align*}

\begin{align*}
\text{Asymmetric unit} & 
\begin{align*}
0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1
\end{align*}
\end{align*}

\begin{align*}
\text{Symmetry Operations} & 
\begin{align*}
(1) \text{ 1} & 
(1 | 0,0,0) \\
\text{ (1 | 0,0,0)' } & \\
(2) \text{ 2' \ 1/4,0,z} & 
(2_z | 1/2,0,0)' \\
(3) \text{ 2' \ 0,y,0} & 
(2_y | 0,0,0)' \\
(4) \text{ 2 \ (1/2,0,0) \ x,0,0} & 
(2_z | 1/2,0,0) \\
(5) \text{ T'} & 
(1 | 0,0,0)' \\
(6) \text{ a \ (1/2,0,0) \ x,y,0} & 
(m_z | 1/2,0,0) \\
(7) \text{ m \ x,0,z} & 
(m_y | 0,0,0) \\
(8) \text{ m' \ 1/4,y,z} & 
(m_z | 1/2,0,0)' \\
\end{align*}
\end{align*}
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>8</th>
<th>l</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(2)</td>
<td>x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4)</td>
<td>x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6)</td>
<td>x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8)</td>
<td>x+1/2,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

4 k m' 1/4, y, z [0,v,w]  
4 j .m. x, 1/2, z [0,v,0]  
4 i .m. x, 0, z [0,v,0]  
4 h .2' 0, y, 1/2 u, 0, w  
4 g .2' 0, y, 0 [u,0,w]  
2 f m'm 2' 1/4, 1/2, z [0,v,0]  
2 e m'm 2' 1/4, 0, z [0,v,0]  
2 d .2'/m 0, 1/2, 1/2 [0,0,0]  
2 c .2'/m 0, 0, 1/2 [0,0,0]  
2 b .2'/m 0, 1/2, 0 [0,0,0]  
2 a .2'/m 0, 0, 0 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1] p2a, 2mm  
Along [1,0,0] p2mm  
Along [0,1,0] p2mg1'  

\[ a^* = \frac{a}{2} \quad b^* = b \]

Origin at 1/4,0,z  
Origin at x,0,0

\[ a^* = -a \quad b^* = c \]

Origin at 0,y,0  
Origin at 0,y,0

51.3.389 - 2 - 767
**Orthorhombic**

### Origin
- at center (2/m') at 2', 2/m'a

### Asymmetric Unit
- $0 \leq x \leq 1/4$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$

### Symmetry Operations

<table>
<thead>
<tr>
<th>Operation</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(1 0,0,0)</td>
</tr>
<tr>
<td>(2) $2'$</td>
<td>1/4,0,z</td>
</tr>
<tr>
<td></td>
<td>(2z 1/2,0,0)</td>
</tr>
<tr>
<td>(3) $2'$</td>
<td>0,y,0</td>
</tr>
<tr>
<td></td>
<td>(2, 0,0,0)</td>
</tr>
<tr>
<td>(4) $2'$</td>
<td>(1/2,0,0) x,0,0</td>
</tr>
<tr>
<td></td>
<td>(2z 1/2,0,0)</td>
</tr>
<tr>
<td>(5) 1</td>
<td>(1 0,0,0)'</td>
</tr>
<tr>
<td>(6) a 1/2</td>
<td>x,y,0</td>
</tr>
<tr>
<td></td>
<td>(mz 1/2,0,0)</td>
</tr>
<tr>
<td>(7) m'</td>
<td>x,0,z</td>
</tr>
<tr>
<td></td>
<td>(my 0,0,0)'</td>
</tr>
<tr>
<td>(8) m</td>
<td>1/4,y,z</td>
</tr>
<tr>
<td></td>
<td>(mz 1/2,0,0)</td>
</tr>
</tbody>
</table>

**Pmm'a**

51.4.390

**mm'm**

P2, /m2/m'2'/a
**Generators selected**  
$(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5)$.

**Positions**

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>8</td>
<td>l</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z [u,v,w]</td>
<td>8</td>
<td>l</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
<td>8</td>
<td>l</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z [u,v,w]</td>
<td>8</td>
<td>l</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>8</td>
<td>l</td>
</tr>
<tr>
<td>4 k m..</td>
<td>1/4,y,z [u,0,0]</td>
<td>4</td>
<td>k</td>
</tr>
<tr>
<td>4 j .m'.</td>
<td>x,1/2,z [u,0,w]</td>
<td>4</td>
<td>j</td>
</tr>
<tr>
<td>4 i .m'.</td>
<td>x,0,z [u,0,w]</td>
<td>4</td>
<td>i</td>
</tr>
<tr>
<td>4 h .2.</td>
<td>0,y,1/2 [0,v,0]</td>
<td>4</td>
<td>h</td>
</tr>
<tr>
<td>4 g .2.</td>
<td>0,y,0 [0,v,0]</td>
<td>4</td>
<td>g</td>
</tr>
<tr>
<td>2 f mm'</td>
<td>1/4,1/2,z [u,0,0]</td>
<td>2</td>
<td>f</td>
</tr>
<tr>
<td>2 e mm'</td>
<td>1/4,0,z [u,0,0]</td>
<td>2</td>
<td>e</td>
</tr>
<tr>
<td>2 d .2/m'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>2</td>
<td>d</td>
</tr>
<tr>
<td>2 c .2/m'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>2</td>
<td>c</td>
</tr>
<tr>
<td>2 b .2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>2</td>
<td>b</td>
</tr>
<tr>
<td>2 a .2/m'</td>
<td>0,0,0 [0,0,0]</td>
<td>2</td>
<td>a</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]** $p_{2a}, 2m'm'$  
  $a^* = a/2$ \ $b^* = b$  
  Origin at 0,0,z

- **Along [1,0,0]** $p2mm1'$  
  $a^* = b$ \ $b^* = c$  
  Origin at x,0,0

- **Along [0,1,0]** $p2mg$  
  $a^* = -a$ \ $b^* = c$  
  Origin at 0,y,0
Pmna'  mmm'  Orthorhombic

51.5.391  P2₁/m/m2/m/a'

Origin  at center (2/m) at 2', 2'/ma'

Asymmetric unit  0 ≤ x ≤ 1/4;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1

Symmetry Operations

(1) 1  
(1 0,0,0)  

(2) 2  
1/4,0,z  
(2z 1/2,0,0)

(3) 2'  
0,y,0  
(2',0,0,0')

(4) 2'  
(1/2,0,0)  
x,0,0  
(2,1/2,0,0)'

(5) T  
(1 0,0,0)'

(6) a'  
(1/2,0,0)  
x,y,0  
(m,1/2,0,0)'

(7) m  
x,0,z  
(m,0,0,0)

(8) m  
1/4,y,z  
(m,1/2,0,0)
### Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2, y, z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2, y, z [u,v,w]</td>
<td>(7) x,y,z [u,v,w]</td>
<td>(8) x+1/2, y, z [u,v,w]</td>
</tr>
<tr>
<td>4 k m..</td>
<td>1/4,y,z [u,0,0]</td>
<td>1/4, y,z [u,0,0]</td>
<td>3/4, y,z [u,0,0]</td>
</tr>
<tr>
<td>4 j .m.</td>
<td>x,1/2,z [0,v,0]</td>
<td>x+1/2,1/2,z [0,v,0]</td>
<td>x+1/2,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>4 i .m.</td>
<td>x,0,z [0,v,0]</td>
<td>x+1/2,0,z [0,v,0]</td>
<td>x+1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 h .2'.</td>
<td>0,y,1/2 [u,0,w]</td>
<td>1/2,y,1/2 [u,0,w]</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 g .2'.</td>
<td>0,y,0 [u,0,w]</td>
<td>1/2,y,0 [u,0,w]</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>2 f mm2</td>
<td>1/4,1/2,z [0,0,0]</td>
<td>3/4,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 e mm2</td>
<td>1/4,0,z [0,0,0]</td>
<td>3/4,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 d .2'/m.</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 c .2'/m.</td>
<td>0,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b .2'/m.</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a .2'/m.</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**  p2mm
  - $a^* = a/2$
  - $b^* = b$
  - Origin at 0,0,z

- **Along [1,0,0]**  p2mm1’
  - $a^* = b$
  - $b^* = c$
  - Origin at x,0,0

- **Along [0,1,0]**  p2mg1’
  - $a^* = -a$
  - $b^* = c$
  - Origin at 0,y,0
Origin at center (2'/m’) at 2’, 2'/m’a

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1 (1 | 0,0,0) (5) (1 | 0,0,0)
(6) a (1/2,0,0) x,y,0 (m_z | 1/2,0,0)

(2) 2 1/4,0,z (2) 2’ 0,y,0 (7) m’ x,0,z (8) m’ 1/4,y,z (m_z | 1/2,0,0)
(2_z | 1/2,0,0) (2_z | 0,0,0)’ (m_y | 0,0,0)’ (m_y | 1/2,0,0)’
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 k m'..</td>
<td>1/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 j m'..</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>4 i m'..</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>4 h .2'..</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 g .2'..</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>2 f m'm'2</td>
<td>1/4,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 e m'm'2</td>
<td>1/4,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d .2'/m'</td>
<td>0,1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 c .2'/m'</td>
<td>0,0,1/2 [u,0,w]</td>
</tr>
<tr>
<td>2 b .2'/m'</td>
<td>0,1/2,0 [u,0,w]</td>
</tr>
<tr>
<td>2 a .2'/m'</td>
<td>0,0,0 [u,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_{2a} 2m'm'  
\(a^* = a/2\)  \(b^* = b\)  
Origin at 1/4,0,z

Along [1,0,0]  p2'm'm'  
\(a^* = a\)  \(b^* = a\)  
Origin at x,0,0

Along [0,1,0]  p2'm'g  
\(a^* = -a\)  \(b^* = -b\)  
Origin at 0,y,0
Pmm'a'

mm'm'

Orthorhombic

51.7.393

P2₁/m2'/m'2'/a'

Origin at center (2'/m') at 2; 2'/m'a'

Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(1 0,0,0)

(2) 2' 1/4,0,z
(2z 1/2,0,0)

(3) 2' 0,y,0
(2y 0,0,0)

(4) 2 (1/2,0,0) x,0,0
(2 (1/2,0,0)

(5) 1
(1 0,0,0)

(6) a' (1/2,0,0) x,y,0
(m 1/2,0,0)

(7) m' x,0,z
(m 0,0,0)

(8) m 1/4,y,z
(m 1/2,0,0)

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Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 l 1 (1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) x+1/2,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(3) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(4) x+1/2,y,z [u,v,w]</td>
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<tr>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
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<tr>
<td>(6) x+1/2,y,z [u,v,w]</td>
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</tr>
<tr>
<td>(7) x,y,z [u,v,w]</td>
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</tr>
<tr>
<td>(8) x+1/2,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 k m..</td>
<td>1/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>1/4,y,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>3/4,y,z [u,0,0]</td>
<td></td>
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<tr>
<td>3/4,y,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 j .m'.</td>
<td>x,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>x+1/2,1/2,z [u,0,w]</td>
<td></td>
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<tr>
<td>x,1/2,z [u,0,w]</td>
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<tr>
<td>x+1/2,1/2,z [u,0,w]</td>
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</tr>
<tr>
<td>4 i .m'.</td>
<td>x,0,z [u,0,0]</td>
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<tr>
<td>x+1/2,0,z [u,0,w]</td>
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<td>x,0,z [u,0,w]</td>
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</tr>
<tr>
<td>x+1/2,0,z [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 h .2'.</td>
<td>0,y,1/2 [u,0,0]</td>
</tr>
<tr>
<td>1/2,y,1/2 [u,0,w]</td>
<td></td>
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<tr>
<td>0,y,1/2 [u,0,w]</td>
<td></td>
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<tr>
<td>1/2,y,1/2 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 g .2'.</td>
<td>0,y,0 [u,0,0]</td>
</tr>
<tr>
<td>1/2,y,0 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>0,y,0 [u,0,w]</td>
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<tr>
<td>1/2,y,0 [u,0,w]</td>
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<td>2 f mm'2'</td>
<td>1/4,1/2,z [u,0,0]</td>
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<td>1/4,0,z [u,0,0]</td>
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<tr>
<td>2 d .2'/m'.</td>
<td>0,1/2,1/2 [u,0,w]</td>
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<td>1/2,1/2,1/2 [u,0,w]</td>
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<td>2 c .2'/m'.</td>
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Symmetry of Special Projections

Along [0,0,1] p2'mm' a* = a/2 b* = b
Origin at 0,0,z

Along [1,0,0] p2mm1' a* = b b* = c
Origin at x,0,0

Along [0,1,0] p2'mg' a* = -a b* = c
Origin at 0,y,0
Origin at center (2/m) at 2,‘2/ma’

Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

1. (1 | 0,0,0)
2. (2' | 1/4,0,z)
3. (3 | 0,y,0)
4. (4' | 1/2,0,0)

5. (5' | 0,0,0)
6. (6a' | 1/2,0,0)
7. (7 | x,0,z)
8. (8 | 1/4,y,z)

Orthorhombic

Pm’ma’
m’mm’

51.8.394 P2_1/m’2/m2’/a’
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>2 e m'm2'</td>
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<td>m'm2'</td>
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<td>0,1/2,0 [0,v,0]</td>
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<td>0,0,0 [0,v,0]</td>
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<td>a</td>
<td>.2/m.</td>
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<td>1/2,0,0 [0,v,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2mm  
\(a^* = a/2\)  \(b^* = b\)  
Origin at 0,0,z

Along [1,0,0] p2'1'm'  
\(a^* = b\)  \(b^* = c\)  
Origin at x,0,0

Along [0,1,0] p21gm  
\(a^* = -a\)  \(b^* = c\)  
Origin at 0,y,0
Origin at center (2/m') at 2, 2/m'a'

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) $1$  
\[ (1 | 0,0,0) \]

(2) $2$  
\[ 1/4,0,z \]
\[ (2z | 1/2,0,0) \]

(3) $2$  
\[ 0,y,0 \]
\[ (2y | 0,0,0) \]

(4) $2$  
\[ (1/2,0,0) \]
\[ x,0,0 \]
\[ (2,1/2,0,0) \]

(5) $\overline{1}$  
\[ (1 | 0,0,0)'^{'} \]

(6) $a'$  
\[ (1/2,0,0) \]
\[ x,y,0 \]
\[ (mz | 1/2,0,0)'^{'} \]

(7) $m'$  
\[ x,0,z \]
\[ (my | 0,0,0)'^{'} \]

(8) $m'$  
\[ 1/4,y,z \]
\[ (mz | 1/2,0,0)'^{'} \]
Continued

Generators selected  (1); t(1,0,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(6) x+1/2,y,z [u,v,w]</td>
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<td>(7) x,y,z [u,v,w]</td>
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<td>(8) x+1/2,y,z [u,v,w]</td>
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<td>4 k m'..</td>
<td>1/4,y,z [0,v,w]</td>
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<td>3/4,y,z [0,v,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'  
\(a^* = a/2\)  \(b^* = b\)
Origin at 0,0,z

Along [1,0,0] p2m'm'  
\(a^* = b\)  \(b^* = c\)
Origin at x,0,0

Along [0,1,0] p2m'g'  
\(a^* = -a\)  \(b^* = c\)
Origin at 0,y,0
Origin at center (2/m) at 2,2/ma

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

**For (0,0,0) + set**

1. 1 (1 0,0,0)
2. 2 1/4,0,z (2,1/2,0,0)
3. 3 0,y,0 (2 0,0,0)
4. 4 (1/2,0,0) x,0,0 (2,1/2,0,0)

5. (5 0,0,0)
6. a (1/2,0,0) x,y,0 (m z 1/2,0,0)
7. m x,0,z (m 0,0,0)
8. m 1/4,y,z (m 1/2,0,0)

**For (0,1,0)' + set**

1. t' (0,1,0) (1 0,1,0)
2. 2' 1/4,1/2,z (2 1/2,1,0)
3. 3' (0,1,0) 0,y,0 (2 0,1,0)
4. 4' (1/2,0,0) x,1/2,0 (2 1/2,1,0)

5. (5 0,1/2,0)
6. n' (1/2,1,0) x,y,0 (m 1/2,1,0)
7. m' x,1/2,z (m 0,1,0)
8. b' (0,1,0) 1/4,y,z (m 1/2,1,0)
Generators selected  
(1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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Symmetry of Special Projections

Along [0,0,1] p2a, 2'2mm'
\( a^* = -b \) \( b^* = a/2 \)
Origin at 0,0,z

Along [1,0,0] p2mm1'
\( a^* = b \) \( b^* = c \)
Origin at x,0,0

Along [0,1,0] p2mg1'
\( a^* = -a \) \( b^* = c \)
Origin at 0,y,0
Orthorhombic

Origin: at center (2/m) at 2, 2/mma

Asymmetric unit:

\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1\]

Symmetry Operations

For \((0,0,0) + \) set

1. \(I \quad (1|0,0,0)\)
2. \(2 \quad \frac{1}{4},0,z\)
   \((2_{z}|1/2,0,0)\)
3. \(2 \quad 0,y,0\)
   \((2_{y}|0,0,0)\)
4. \(2 \quad (1/2,0,0) \times 0,0\)
   \((2_{x}|1/2,0,0)\)
5. \(\bar{1} \quad (1|0,0,0)\)
6. \(a \quad (1/2,0,0)\)
   \((m_{x}|1/2,0,0)\)
7. \(m \quad x,0,z\)
   \((m_{y}|0,0,0)\)
8. \(m \quad 1/4,y,z\)
   \((m_{z}|1/2,0,0)\)

For \((0,0,1)') + \) set

1. \(t' \quad (0,0,1)\)
   \((1|0,0,1)\)
2. \(2' \quad (0,0,1) \times \frac{1}{4},0,z\)
   \((2_{z}|1/2,0,1)'\)
3. \(2' \quad 0,y,1/2\)
   \((2_{y}|0,0,1)'\)
4. \(2' \quad (1/2,0,0) \times 0,1/2\)
   \((2_{x}|1/2,0,1)'\)
5. \(\bar{1}' \quad 0,0,1/2\)
   \((1|0,0,1)'\)
6. \(a' \quad (1/2,0,0)\)
   \((m_{x}|1/2,0,1)'\)
7. \(c' \quad (0,0,1) \times 0,z\)
   \((m_{y}|0,0,1)'\)
8. \(c' \quad (0,0,1) \times 1/4,y,z\)
   \((m_{z}|1/2,0,1)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>16 l</td>
<td>(1) x,y,z [u,v,w] (2) x+1/2,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w] (6) x+1/2,y,z [u,v,w] (7) x,y,z [u,v,w] (8) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 k m..</td>
<td>1/4,y,z [u,0,0] 3/4,y,z [u,0,0] 3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 j m.</td>
<td>x,1/2,z [0,v,0] x+1/2,1/2,z [0,v,0] x+1/2,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>8 i m.</td>
<td>x,0,z [0,v,0] x+1/2,0,z [0,v,0] x+1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 h .2'</td>
<td>0,y,1/2 [u,0,w] 1/2,y,1/2 [u,0,w] 1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 g .2.</td>
<td>0,y,0 [0,v,0] 1/2,y,0 [0,v,0] 1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 f mm2</td>
<td>1/4,1/2,z [0,0,0] 3/4,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 e mm2</td>
<td>1/4,0,z [0,0,0] 3/4,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 d .2'/m.</td>
<td>0,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2'/m.</td>
<td>0,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b .2'/m.</td>
<td>0,1/2,0 [0,v,0] 1/2,1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>4 a .2'/m.</td>
<td>0,0,0 [0,v,0] 1/2,0,0 [0,v,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mm1'     Along [1,0,0]  p2mm1'     Along [0,1,0]  p2mm1'
\( \mathbf{a}^* = \mathbf{a}/2 \)   \( \mathbf{b}^* = \mathbf{b} \)   \( \mathbf{a}^* = \mathbf{a} \) \( \mathbf{b}^* = \mathbf{c} \)
Origin at 0,0,z     Origin at x,0,0     Origin at 0,y,0
Origin at center (2/m) at 2, 2/ma

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1
Symmetry Operations

For (0,0,0) + set

(1) \( T \) (0,0,0)
(2) \( 2 \) \( \frac{1}{4}, 0, z \)
(3) \( 2 \) 0,0,0
(4) \( 2 \left( \frac{1}{2}, 0, 0 \right) \) \( x, 0, 0 \)

(5) \( \bar{T} \) (1/0,0,0)
(6) \( a \left( \frac{1}{2}, 0, 0 \right) \) \( x, y, 0 \)
(7) \( m \) \( x, 0, z \)
(8) \( m \left( \frac{1}{4}, y, z \right) \)

For (0,1,0)' + set

(1) \( t' \) (0,1,0)
(2) \( 2' \) \( \frac{1}{4}, 0, z \)
(3) \( 2' \) (0,0,0)
(4) \( 2' \left( \frac{1}{2}, 0, 0 \right) \) \( x, 0, 0 \)

(5) \( \bar{T} \) (0,1,0)'
(6) \( n' \left( \frac{1}{2}, 0, 0 \right) \) \( x, y, 0 \)
(7) \( m' \) \( x, 0, z \)
(8) \( b' \) (0,0,0)

Generators selected (1); (0,1,0); (1,0,0); (0,0,1); (2); (3); (5).

Positions

Multiplicty, Wyckoff letter, Site Symmetry.

Coorinates

(0,0,0) + (0,1,0)'

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 l 1</td>
<td>(0,0,0) + (0,1,0)' +</td>
<td></td>
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<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>x+1/2, y, z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) ( x+1/2, y, z \ [u,v,w] )</td>
<td>( x+1/2, y, z \ [u,v,w] )</td>
<td>( x+1/2, y, z \ [u,v,w] )</td>
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<tr>
<td>(5) ( x, y, z \ [u,v,w] )</td>
<td>( x, y, z \ [u,v,w] )</td>
<td>( x, y, z \ [u,v,w] )</td>
</tr>
<tr>
<td>8 k m..</td>
<td>( 1/4, y, z \ [u,0,0] )</td>
<td>( 1/4, y, z \ [u,0,0] )</td>
</tr>
<tr>
<td>8 j m'.</td>
<td>( x, 1/2, z \ [u,0,0] )</td>
<td>( x, 1/2, z \ [u,0,0] )</td>
</tr>
<tr>
<td>8 i .m.</td>
<td>( x, 0, z \ [0,v,0] )</td>
<td>( x, 0, z \ [0,v,0] )</td>
</tr>
<tr>
<td>8 h .2'</td>
<td>( 0, y, 1/2 \ [u,0,0] )</td>
<td>( 1/2, y, 1/2 \ [u,0,0] )</td>
</tr>
<tr>
<td>8 g .2.</td>
<td>( 0, y, 0 \ [0,v,0] )</td>
<td>( 1/2, y, 0 \ [0,v,0] )</td>
</tr>
<tr>
<td>4 f mm'2'</td>
<td>( 1/4, 1/2, z \ [u,0,0] )</td>
<td>( 3/4, 1/2, z \ [u,0,0] )</td>
</tr>
<tr>
<td>4 e mm2</td>
<td>( 1/4, 0, z \ [0,0,0] )</td>
<td>( 3/4, 0, z \ [0,0,0] )</td>
</tr>
<tr>
<td>4 d .2'/m'.</td>
<td>( 0, 1/2, 1/2 \ [u,0,0] )</td>
<td>( 1/2, 1/2, 1/2 \ [u,0,0] )</td>
</tr>
<tr>
<td>4 c .2'/m</td>
<td>( 0, 0, 1/2 \ [0,0,0] )</td>
<td>( 1/2, 0, 1/2 \ [0,0,0] )</td>
</tr>
<tr>
<td>4 b .2/m'</td>
<td>( 0, 1/2, 0 \ [0,0,0] )</td>
<td>( 1/2, 1/2, 0 \ [0,0,0] )</td>
</tr>
<tr>
<td>4 a .2/m</td>
<td>( 0, 0, 0 \ [0,0,0] )</td>
<td>( 1/2, 0, 0 \ [0,0,0] )</td>
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</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1]  p2mm1'  
\( \mathbf{a}^* = \frac{\mathbf{a}}{2} \quad \mathbf{b}^* = \mathbf{b} \)
Origin at 0,0,z

Along [1,0,0]  p2mm1'  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)
Origin at x,0,0

Along [0,1,0]  p2mg1'  
\( \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c} \)
Origin at 0,y,0
Origin at center (2/m) at 2, 2/m, ma

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

1. \( \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \)
2. \( \begin{pmatrix} 2' \\ 1/4,0,z \end{pmatrix} \)
3. \( \begin{pmatrix} 2' \\ 0,y,0 \end{pmatrix} \)
4. \( \begin{pmatrix} 2 \end{pmatrix} \)

For (0,1,0)' + set

1. \( \begin{pmatrix} t' \\ 0,1,0 \end{pmatrix} \)
2. \( \begin{pmatrix} 2 \end{pmatrix} \)
3. \( \begin{pmatrix} 2 \end{pmatrix} \)
4. \( \begin{pmatrix} 2' \end{pmatrix} \)

For (0,0,0)' + set

1. \( \begin{pmatrix} 5 \end{pmatrix} \)
2. \( \begin{pmatrix} 6 \end{pmatrix} \)
3. \( \begin{pmatrix} 7 \end{pmatrix} \)
4. \( \begin{pmatrix} 8 \end{pmatrix} \)

1. \( \begin{pmatrix} 1 \end{pmatrix} \)
2. \( \begin{pmatrix} 2 \end{pmatrix} \)
3. \( \begin{pmatrix} 2 \end{pmatrix} \)
4. \( \begin{pmatrix} 2 \end{pmatrix} \)

1. \( \begin{pmatrix} 5 \end{pmatrix} \)
2. \( \begin{pmatrix} 6 \end{pmatrix} \)
3. \( \begin{pmatrix} 7 \end{pmatrix} \)
4. \( \begin{pmatrix} 8 \end{pmatrix} \)
Generators selected

(1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>u,v,w</td>
<td>16 l 1</td>
</tr>
<tr>
<td>(0,1,0)</td>
<td>u,v,w</td>
<td>4 f m'm'2</td>
</tr>
<tr>
<td>(0,2,0)</td>
<td>u,v,w</td>
<td>4 e m'm'2</td>
</tr>
<tr>
<td>(1,0,0)</td>
<td>u,v,w</td>
<td>4 d .2'/m'</td>
</tr>
<tr>
<td>(1,1,0)</td>
<td>u,v,w</td>
<td>4 c .2'/m'</td>
</tr>
<tr>
<td>(1,2,0)</td>
<td>u,v,w</td>
<td>4 b .2'/m'</td>
</tr>
<tr>
<td>(2,0,0)</td>
<td>u,v,w</td>
<td>4 a .2'/m'</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_2 mm
\( a^* = -a/2 \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0]  p_{2a} 2 mm
\( a^* = b \quad b^* = c \)
Origin at x,0,0

Along [0,1,0]  p_{2mg} 1'
\( a^* = -a \quad b^* = c \)
Origin at 0,y,0
**Origin** at center (2'/m) at 2', 2'/ma'

**Asymmetric unit**

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

**Symmetry Operations**

For (0,0,0) + set

1. $\text{I} (0,0,0)$
2. $\text{I} 1/4,0,z (2_z 1/2,0,0)$
3. $2' 0,y,0 (2_y 0,0,0)$
4. $2' (1/2,0,0) x,0,0 (2_x 1/2,0,0)$
5. $\text{a'} (1/2,0,0) x,y,0 (m_z 1/2,0,0)$
6. $m 0,z (m_z 0,0,0)$
7. $m' x,0,z (m_z 0,0,0)$
8. $b' (0,1,0) 1/4,y,z (m_z 1/2,1,0)$

For (0,1,0) + set

1. $t' (0,1,0) (1,0,0)$
2. $t' 1/4,1/2,z (2_z 1/2,1,0)$
3. $2 (0,1,0) 0,y,0 (2_x 0,1,0)$
4. $2 (1/2,0,0) x,1/2,0 (2_x 1/2,1,0)$
5. $\text{n} (1/2,1,0) x,y,0 (m_z 1/2,1,0)$
6. $m' x,1/2,z (m_y 0,1,0)$
7. $b' (0,1,0) 1/4,y,z (m_x 1/2,1,0)$
8. $b' (0,1,0) 1/4,y,z (m_x 1/2,1,0)$
Generators selected  (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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</tr>
<tr>
<td>8 k m..</td>
<td>8</td>
<td>1/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 j .m'.</td>
<td>8</td>
<td>x+1/2,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>8 i .m.</td>
<td>8</td>
<td>x+1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 h .2'</td>
<td>8</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 g .2'</td>
<td>8</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 f mm'2'</td>
<td>4</td>
<td>1/4,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>4 e mm2</td>
<td>4</td>
<td>1/4,0,z [0,0,0]</td>
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<tr>
<td>4 d .2'/m'</td>
<td>4</td>
<td>0,1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 c .2'/m</td>
<td>4</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b .2'/m'</td>
<td>4</td>
<td>0,1/2,0 [u,0,w]</td>
</tr>
<tr>
<td>4 a .2'/m'</td>
<td>4</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a},2mm  
Along [1,0,0] p 2mm1'  
Along [0,1,0] p2mg1'

\( \mathbf{a}^* = -b \quad \mathbf{b}^* = a/2 \quad \mathbf{c}^* = c \)

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center \((2/m)\) at \(2'2/ma'\)

Asymmetric unit \(0 < x < 1/4; \ 0 < y < 1/2; \ 0 < z < 1\)

Symmetry Operations

For \((0,0,0)\) + set

1. \(T\) \((1|0,0,0)\)
2. \(2'\) \(1/4,0,z\) \((2_z|1/2,0,0)\)
3. \(T\) \(0,y,0\) \((2_y|0,0,0)\)
4. \(2'\) \(1/2,0,0\) \(x,0,0\) \((2_x|1/2,0,0)\)

5. \(\bar{T}\) \((1|0,0,0)\)
6. \(a'\) \((1/2,0,0)\) \(x,y,0\) \((m_z|1/2,0,0)\)
7. \(m\) \(x,0,z\) \((m_y|0,0,0)\)
8. \(m'\) \(1/4,y,z\) \((m_x|1/2,0,0)\)

For \((0,1,0)'\) + set

1. \(t'\) \((0,1,0)\)
2. \(2\) \(1/4,1/2,z\) \((2_z|1/2,1,0)\)
3. \(2'\) \((0,1,0)\) \(0,y,0\) \((2_y|0,1,0)\)
4. \(2\) \((1/2,0,0)\) \(x,1/2,0\) \((2_x|1/2,1,0)\)

5. \(\bar{T}\) \(0,1/2,0\)
6. \(n\) \((1/2,1,0)\) \(x,y,0\) \((m_z|1/2,1,0)\)
7. \(m'\) \(x,1/2,z\) \((m_y|0,1,0)\)
8. \(b\) \((0,1,0)\) \(1/4,y,z\) \((m_x|1/2,1,0)\)
Generators selected  
(1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicities, 
Wyckoff letters, 
Site Symmetry.

 Coordinates

(0,0,0) + (0,1,0)' +

| 16 | l | 1 | (1) x,y,z [u,v,w] | (2) x+1/2,y,z [u,v,w] | (3) x,y,z [u,v,w] | (4) x+1/2,y,z [u,v,w] |
|---|---|---|---|---|---|---|---|
| 8 | k | m' | 1/4, y,z [0,v,w] | 1/4, y,z [0,v,w] | 3/4, y,z [0,v,w] | 3/4, y,z [0,v,w] |
| 8 | j | m' | x,1/2,z [u,0,w] | x+1/2,1/2,z [u,0,w] | x,1/2,z [u,0,w] | x+1/2,1/2,z [u,0,w] |
| 8 | i | m | x,0,z [0,v,0] | x+1/2,0,z [0,v,0] | x,0,z [0,v,0] | x+1/2,0,z [0,v,0] |
| 8 | h | .2. | 0,y,1/2 [0,v,0] | 1/2, y,1/2 [0,v,0] | 0,y,1/2 [0,v,0] | 1/2, y,1/2 [0,v,0] |
| 8 | g | .2. | 0,y,0 [0,v,0] | 1/2, y,0 [0,v,0] | 0,y,0 [0,v,0] | 1/2, y,0 [0,v,0] |
| 4 | f | m' m' | 1/4,1/2,z [0,0,w] | 3/4,1/2,z [0,0,w] | 3/4,1/2,z [0,0,w] | 3/4,1/2,z [0,0,w] |
| 4 | e | m' m' | 1/4,0,z [0,v,0] | 3/4,0,z [0,v,0] | 3/4,0,z [0,v,0] | 3/4,0,z [0,v,0] |
| 4 | d | .2/m' | 0,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |
| 4 | c | .2/m | 0,0,1/2 [0,v,0] | 1/2,0,1/2 [0,v,0] | 1/2,0,1/2 [0,v,0] | 1/2,0,1/2 [0,v,0] |
| 4 | b | .2/m' | 0,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 4 | a | .2/m | 0,0,0 [0,v,0] | 1/2,0,0 [0,v,0] | 1/2,0,0 [0,v,0] | 1/2,0,0 [0,v,0] |

Symmetry of Special Projections

Along [0,0,1] p2a 2'm' Along [1,0,0] p2a 2'm' Along [0,1,0] p2mg1' 
\[ a^* = -b \quad b^* = a/2 \] \[ a^* = b \quad b^* = c \] \[ a^* = -a \quad b^* = c \]

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin: at center (\(2'/m\)) at \(2',2'/ma'\)

Asymmetric unit:  
\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1\]

Symmetry Operations:

For \((0,0,0)\) + set:

1. \(1\) \[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\]
2. \(2'\) \[\begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{4} & 0 & z \end{pmatrix}\]
3. \(2'\) \[\begin{pmatrix} 0 & y & 0 \\ \frac{1}{4} & 0 & z \end{pmatrix}\]
4. \(2\) \[\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ z & 0 & 0 \end{pmatrix}\]

For \((0,0,1)\) + set:

1. \(t'\) \[\begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{4} & 0 & z \end{pmatrix}\]
2. \(a\) \[\begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\]
3. \(m\) \[\begin{pmatrix} 0 & 0 & z \\ 0 & 0 & 0 \end{pmatrix}\]
4. \(m'\) \[\begin{pmatrix} 1/4 & y & z \\ 0 & 0 & 0 \end{pmatrix}\]

For \((0,0,0)\)' + set:

1. \(t'\) \[\begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{4} & 0 & z \end{pmatrix}\]
2. \(a\) \[\begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\]
3. \(m\) \[\begin{pmatrix} 0 & 0 & z \\ 0 & 0 & 0 \end{pmatrix}\]
4. \(m'\) \[\begin{pmatrix} 1/4 & y & z \\ 0 & 0 & 0 \end{pmatrix}\]
### Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
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<td>(0,0,0) +</td>
</tr>
<tr>
<td>16 l</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(3) x,y,z [u,v,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<td>(7) x,y,z [u,v,w]</td>
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<tr>
<td>8 k</td>
<td>1/4,y,z [u,v,0]</td>
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<tr>
<td>8 i</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 f</td>
<td>1/4,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>4 e</td>
<td>1/4,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>0,1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>0,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p2mm1'
  - \( a^* = a/2 \)
  - \( b^* = b \)
  - Origin at 0,0,z

- **Along [1,0,0]**: p2a'2mm
  - \( a^* = -c \)
  - \( b^* = b \)
  - Origin at x,0,0

- **Along [0,1,0]**: p2mg1'
  - \( a^* = -a \)
  - \( b^* = c \)
  - Origin at 0,y,0

---

51.16.402 - 2 - 794
**Orthorhombic**

**P2c mm'a**

51.17.403

<table>
<thead>
<tr>
<th>Origin</th>
<th>at center (2/m') at 2, 2/m'a</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asymmetric unit</td>
<td>0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

For (0,0,0) + set

1. **1 (0,0,0)**
   - (1) 1
   - (2) 2' 1/4,0,z
   - (3) 2 0,y,0
   - (4) 2' (1/2,0,0) x,0,0
   - (5) 1 x,0,0
   - (6) a (1/2,0,0) x,y,0
   - (7) m' x,0,z
   - (8) m 1/4,y,z

For (0,0,1)' + set

1. **1 (0,0,1)**
   - (1) t' (0,0,1)
   - (2) 2 (0,0,1) 1/4,0,z
   - (3) 2' 0,y,1/2
   - (4) 2 (1/2,0,0) x,0,1/2
   - (5) 0,0,1/2
   - (6) a' (1/2,0,0) x,y,1/2
   - (7) c (0,0,1) x,0,z
   - (8) c' (0,0,1) 1/4,y,z

For (0,0,1) + set

1. **1 (0,0,1)**
   - (1) t (0,0,1)
   - (2) 2 (0,0,1) 1/4,0,z
   - (3) 2' 0,y,1/2
   - (4) 2 (1/2,0,0) x,0,1/2
   - (5) 0,0,1/2
   - (6) a' (1/2,0,0) x,y,1/2
   - (7) c (0,0,1) x,0,z
   - (8) c' (0,0,1) 1/4,y,z

51.17.403 - 1 - 795
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' +</td>
<td></td>
</tr>
<tr>
<td>16  l  1 (1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>8  k  m.. 1/4,y,z [u,0,0]</td>
<td>1/4,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,y,z [u,0,0]</td>
</tr>
<tr>
<td>8  j  .m'. x,1/2,z [u,0,w]</td>
<td>x+1/2,1/2,z [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>8  i  .m'. x,0,z [u,0,w]</td>
<td>x+1/2,0,z [u,0,w]</td>
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<td></td>
<td>x,0,z [u,0,w]</td>
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<tr>
<td></td>
<td>x+1/2,0,z [u,0,w]</td>
</tr>
<tr>
<td>8  h  .2'. 0,y,1/2 [u,0,w]</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8  g  .2. 0,y,0 [0,v,0]</td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4  f  mm'2' 1/4,1/2,z [u,0,0]</td>
<td>3/4,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>4  e  mm'2' 1/4,0,z [u,0,0]</td>
<td>3/4,0,z [u,0,0]</td>
</tr>
<tr>
<td>4  d  .2'/m' 0,1/2,1/2 [u,0,w]</td>
<td>1/2,1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4  c  .2'/m' 0,0,1/2 [u,0,w]</td>
<td>1/2,0,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4  b  .2'/m' 0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4  a  .2/m'. 0,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm1`
  \[a^* = a/2 \quad b^* = b\]
  Origin at 0,0,z

- Along [1,0,0] p2mm1`
  \[a^* = b \quad b^* = c\]
  Origin at x,0,0

- Along [0,1,0] p2m'2mg
  \[a^* = -a \quad b^* = c\]
  Origin at 0,y,0
Origin at center (2/m'') at 2'1'2/m'a

Asymmetric unit 0 < x < 1/4; 0 < y < 1/2; 0 < z < 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 1/4,0,z
(2 | 1/2,0,0)

(3) 2' 0,y,0
(2' | 0,0,0)

(4) 2' (1/2,0,0) x,0,0
(2' | 1/2,0,0)

(5) 1
(1 | 0,0,0)

(6) a (1/2,0,0) x,y,0
(mz | 1/2,0,0)

(7) m' x,0,z
(m | 0,0,0)

(8) m' 1/4,y,z
(m | 1/2,0,0)

For (0,0,1) + set

(1) t' (0,0,1)
(1 | 0,0,1)

(2) 2' (0,0,1) 1/4,0,z
(2' | 1/2,0,1)

(3) 2 0,y,1/2
(2 | 0,0,1)

(4) 2 (1/2,0,0) x,0,1/2
(2 | 1/2,0,1)

(5) 1
(1 | 0,0,0)

(6) a' (1/2,0,0) x,y,1/2
(mz | 1/2,0,1)

(7) c (0,0,1) x,0,z
(m | 0,0,1)

(8) c (0,0,1) 1/4,y,z
(m | 1/2,0,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,1) ' +</td>
</tr>
<tr>
<td>16 l 1 (1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 k m'. 1/4,y,z [0,v,w]</td>
<td>1/4,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 j .m'. x,1/2,z [u,0,w]</td>
<td>x+1/2,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>8 i .m'. x,0,z [u,0,w]</td>
<td>x+1/2,0,z [u,0,w]</td>
</tr>
<tr>
<td>8 h .2. 0,y,1/2 [0,v,0]</td>
<td>1/2,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 g .2'. 0,y,0 [u,0,w]</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 f m'm'2 1/4,1/2,z [0,0,w]</td>
<td>3/4,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e m'm'2 1/4,0,z [0,0,w]</td>
<td>3/4,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 d .2/m'. 0,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2/m'. 0,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b .2'/m'. 0,1/2,0 [u,0,w]</td>
<td>1/2,1/2,0 [u,0,w]</td>
</tr>
<tr>
<td>4 a .2'/m'. 0,0,0 [u,0,w]</td>
<td>1/2,0,0 [u,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1'  
\[ a^* = a/2 \quad b^* = b \]  
Origin at 0,0,0  
Along [1,0,0] p2a* 2'mm'  
\[ a^* = -c \quad b^* = b \]  
Origin at x,0,0  
Along [0,1,0] p2a* 2'm'g'  
\[ a^* = -a \quad b^* = c \]  
Origin at 0,y,1/2
Origin at center \((2'/m\) at 2, 2'/ma\)

Asymmetric unit \(0 \leq x \leq 1/4;\quad 0 \leq y \leq 1/2;\quad 0 \leq z \leq 1\)
Symmetry Operations

For \((0,0,0) + \text{ set}\)

\[
\begin{align*}
(1) & \quad 1 & (2) & \quad 2' \quad 1/4,0,z & (3) & \quad 2' \quad 0,y,0 & (4) & \quad 2 \quad (1/2,0,0) \quad x,0,0 \\
& \quad (1|0,0,0) & & (2|1/2,0,0)' & & (2|0,0,0)' & & (2|1/2,0,0) \\
(5) & \quad \overline{T} \quad \overline{1} & (6) & \quad a \quad (1/2,0,0) \quad x,y,0 & (7) & \quad m \quad x,0,z & (8) & \quad m' \quad 1/4,y,z \\
& \quad (\overline{T} \quad 0,0,0)' & & (m|1/2,0,0) & & (m|0,0,0) & & (m|1/2,0,0)' \\
\end{align*}
\]

For \((0,1,0)' + \text{ set}\)

\[
\begin{align*}
(1) & \quad t' \quad (0,1,0) & (2) & \quad 2 \quad 1/4,1/2,z & (3) & \quad 2 \quad (0,1,0) \quad 0,y,0 & (4) & \quad 2' \quad (1/2,0,0) \quad x,1/2,0 \\
& \quad (1|0,1,0)' & & (2|1/2,1,0) & & (2|0,1,0) & & (2|1/2,1,0)' \\
(5) & \quad \overline{T} \quad 0,1/2,0 & (6) & \quad n' \quad (1/2,1,0) \quad x,y,0 & (7) & \quad m' \quad x,1/2,z & (8) & \quad b \quad (0,1,0) \quad 1/4,y,z \\
& \quad (\overline{T} \quad 0,1,0)' & & (m|1/2,1,0)' & & (m|0,1,0)' & & (m|1/2,1,0) \\
\end{align*}
\]

Generators selected \((1); \; t(1,0,0); \; t'(0,1,0); \; t'(0,0,1); \; (2); \; (3); \; (5).\)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
16 & \quad l \quad 1 \quad (1) & \quad x,y,z \quad [u,v,w] & (2) & \quad x+1/2,y,z \quad [u,v,w] & (3) & \quad x,y,z \quad [u,v,w] & (4) & \quad x+1/2,y,z \quad [u,v,w] \\
& \quad (5) & \quad x,y,z \quad [u,v,w] & (6) & \quad x+1/2,y,z \quad [u,v,w] & (7) & \quad x,y,z \quad [u,v,w] & (8) & \quad x+1/2,y,z \quad [u,v,w] \\
8 & \quad k \quad m'.. \quad 1/4,y,z \quad [0,v,w] & 1/4,y,z \quad [0,v,w] & 3/4,y,z \quad [0,v,w] & 3/4,y,z \quad [0,v,w] \\
8 & \quad j \quad .m'. \quad x,1/2,z \quad [u,0,w] & x+1/2,1/2,z \quad [u,0,w] & x,1/2,z \quad [u,0,w] & x+1/2,1/2,z \quad [u,0,w] \\
8 & \quad i \quad .m. \quad x,0,z \quad [0,v,0] & x+1/2,0,z \quad [0,v,0] & x,0,z \quad [0,v,0] & x+1/2,0,z \quad [0,v,0] \\
8 & \quad h \quad .2. \quad 0,y,1/2 \quad [0,v,0] & 1/2,y,1/2 \quad [0,v,0] & 0,y,1/2 \quad [0,v,0] & 1/2,y,1/2 \quad [0,v,0] \\
8 & \quad g \quad .2'. \quad 0,y,0 \quad [u,0,w] & 1/2,y,0 \quad [u,0,w] & 0,y,0 \quad [u,0,w] & 1/2,y,0 \quad [u,0,w] \\
4 & \quad f \quad m'm'2 \quad 1/4,1/2,z \quad [0,0,w] & 3/4,1/2,z \quad [0,0,w] \\
4 & \quad e \quad m'm'2 \quad 1/4,0,z \quad [0,v,0] & 3/4,0,z \quad [0,v,0] \\
4 & \quad d \quad .2/m'. \quad 0,1/2,1/2 \quad [0,0,0] & 1/2,1/2,1/2 \quad [0,0,0] \\
4 & \quad c \quad .2/m. \quad 0,0,1/2 \quad [0,v,0] & 1/2,0,1/2 \quad [0,v,0] \\
4 & \quad b \quad .2'/m'. \quad 0,1/2,0 \quad [u,0,w] & 1/2,1/2,0 \quad [u,0,w] \\
4 & \quad a \quad .2'/m. \quad 0,0,0 \quad [0,0,0] & 1/2,0,0 \quad [0,0,0] \\
\end{align*}
\]
Symmetry of Special Projections

Along $[0,0,1]$  p2mm1'
\[ a^* = a/2 \quad b^* = b \]
Origin at 0,0,z

Along $[1,0,0]$  p\{1\} 2mm
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along $[0,1,0]$  p2mg1'
\[ a^* = -a \quad b^* = c \]
Origin at 0,y,0
Origin at $\overline{1}$ on n1a

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) \( \mathbf{1} \)
(2) \( 2 \quad 1/4,0,z \quad (2z\mid1/2,0,0) \)
(3) \( 2 \quad (0,1/2,0) \quad 1/4,y,1/4 \quad (2z\mid1/2,1/2,1/2) \)
(4) \( 2 \quad x,1/4,1/4 \quad (2z\mid0,1/2,1/2) \)

(5) \( \overline{1} \quad 0,0,0 \quad (1\mid0,0,0) \)
(6) \( a \quad (1/2,0,0) \quad x,y,0 \quad (m_{\parallel}1/2,0,0) \)
(7) \( n \quad (1/2,0,1/2) \quad x,1/4,z \quad (m_{\parallel}1/2,1/2,1/2) \)
(8) \( n \quad (0,1/2,1/2) \quad 0,y,z \quad (m_{\parallel}0,1/2,1/2) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 d 2..</td>
<td>x,1/4,1/4 [u,0,0]</td>
<td>x+1/2,3/4,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 c ..2</td>
<td>1/4,0,z [0,0,w]</td>
<td>1/4,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,0,1/2 [u,v,w]</td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,1,0]  c_2,2'm'm'
Along [1,0,0]  c_2,2'm'm'
Along [0,0,1]  c_2,2'm'm'

\( a^* = -\mathbf{b} \quad \mathbf{b}^* = \mathbf{a}/2 \)

Origin at 1/4,0,z

Origin at x,0,0

Origin at 1/4,y,1/4
Origin at $\overline{1}1'$ on n1a1'

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y < 1/4; \quad 0 \leq z < 1/2$

Symmetry Operations

For 1 + set

1. $1 (0,0,0)$
2. $2 \frac{1}{4},0,0$ to $2 \frac{1}{2},0,0$
3. $2 (0,1/2,0) \frac{1}{4},y,1/4$
4. $2x,1/4,1/4$

5. $0,0,0$
6. $a (1/2,0,0) x,y,0$
7. $n (1/2,0,1/2) x,1/4,z$
8. $n (0,1/2,1/2) 0,y,z$

For 1' + set

1. $1' (0,0,0)$
2. $2' \frac{1}{4},0,0$ to $2' \frac{1}{2},0,0$
3. $2' (0,1/2,0) \frac{1}{4},y,1/4$
4. $2' x,1/4,1/4$

5. $0,0,0'$
6. $a' (1/2,0,0) x,y,0$
7. $n' (1/2,0,1/2) x,1/4,z$
8. $n' (0,1/2,1/2) 0,y,z$
Continued

**Generators selected**
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1+</td>
<td>1' +</td>
</tr>
<tr>
<td>8  e  11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y+1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4  d  2..1'</td>
<td>x,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,3/4,1/4 [0,0,0]</td>
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<td>x,3/4,3/4 [0,0,0]</td>
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<td>x+1/2,1/4,3/4 [0,0,0]</td>
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<tr>
<td>4  c  ..21'</td>
<td>1/4,0,z [0,0,0]</td>
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<td>1/4,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
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<td>3/4,0,z [0,0,0]</td>
</tr>
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<td>3/4,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4  b  ~1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
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<td></td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4  a  ~1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [0,0,0]</td>
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</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2mg1'  
  \(a^* = -b\)  \(b^* = a/2\)  
  Origin at 1/4,0,z

- Along [1,0,0]  c2mm1'  
  \(a^* = b\)  \(b^* = c\)  
  Origin at x,0,0

- Along [0,1,0]  c2mm1'  
  \(a^* = c\)  \(b^* = a\)  
  Origin at 1/4,y,1/4

---

**Page Dimensions:** 612.0x792.0

**52.2.407  Pnna1'**
Origin at $\bar{1}$ on n'1a

Asymmetric unit: $0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$
   \hspace{1cm} (2) $2' \quad (1/4,0,z)$
   \hspace{1cm} (3) $2' \quad (0,1/2,0) \quad (1/4,y,1/4)$
   \hspace{1cm} (4) $2 \quad (x,1/4,1/4)$
   \hspace{1cm} (5) $\bar{1} \quad (0,0,0)$
   \hspace{1cm} (2' \quad (1/2,0,0))$
   \hspace{1cm} (2' \quad (1/2,1/2,1/2))$
   \hspace{1cm} (2' \quad (0,1/2,1/2))$
   \hspace{1cm} (6) $a \quad (1/2,0,0) \quad x,y,0$
   \hspace{1cm} (7) $n \quad (1/2,0,1/2) \quad x,1/4,z$
   \hspace{1cm} (8) $n' \quad (0,1/2,1/2) \quad 0,y,z$
   \hspace{1cm} (m_\parallel \quad 1/2,0,0)$
   \hspace{1cm} (m_\parallel \quad 1/2,1/2,1/2)$
   \hspace{1cm} (m_\parallel \quad 0,1/2,1/2)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1 (1) x,y,z [u,v,w]</td>
<td>(2) x +1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) x +1/2,y +1/2,z +1/2 [u,v,w]</td>
<td>(4) x,y +1/2,z +1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) x +1/2,y,z [u,v,w]</td>
<td>(6) x +1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>(7) x +1/2,y +1/2,z +1/2 [u,v,w]</td>
<td>(8) x,y +1/2,z +1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 d 2.. x,1/4,1/4 [u,0,0]</td>
<td>(3) x +1/2,3/4,1/4 [u,0,0]</td>
</tr>
<tr>
<td>(4) x +1/2,3/4,1/4 [u,0,0]</td>
<td>(5) x +1/2,1/4,3/4 [u,0,0]</td>
</tr>
<tr>
<td>4 c .2' 1/4,0,z [u,v,0]</td>
<td>(6) 1/4,1/2,z +1/2 [u,v,0]</td>
</tr>
<tr>
<td>(7) 1/4,1/2,z +1/2 [u,v,0]</td>
<td>(8) 3/4,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 b 1' 0,0,1/2 [0,0,0]</td>
<td>(9) 1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>(10) 1/2,0,1/2 [0,0,0]</td>
<td>(11) 0,1/2,0 [0,0,0]</td>
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<tr>
<td>4 a 1' 0,0,0 [0,0,0]</td>
<td>(12) 1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>(13) 1/2,1/2,1/2 [0,0,0]</td>
<td>(14) 0,1/2,1/2 [0,0,0]</td>
</tr>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p_{2b}.2m'g'</th>
<th>Along [1,0,0] c 2mm</th>
<th>Along [0,1,0] c_{p'} 2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = -b  b^* = a/2</td>
<td>a^* = b  b^* = c</td>
<td>a^* = -a  b^* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 1/4,y,1/4</td>
</tr>
</tbody>
</table>
Origin at \(\overline{1}\) on \(n1\)

Asymmetric unit \(0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

1. \(T\) \(1,0,0\)
2. \(2'\) \(1/4,0,z\)
3. \(2\) \((0,1/2,0) \quad 1/4,y,1/4\)
4. \(2'\) \(0,x,1/4,1/4\)
5. \(T'\) \(0,0,0\)
6. \(a\) \((1/2,0,0) \quad x,y,0\)
7. \(n'\) \((1/2,0,1/2) \quad x,1/4,z\)
8. \(n\) \((0,1/2,1/2) \quad 0,y,z\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<tr>
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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1 (1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(6) x+1/2,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 d 2'.</td>
<td>x,1/4,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,3/4,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,3/4,3/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/4,3/4 [0,v,w]</td>
</tr>
<tr>
<td>4 c 2'.</td>
<td>1/4,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/4,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b 1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [0,0,0]</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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<td></td>
<td>0,1/2,0 [0,0,0]</td>
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<tr>
<td>4 a 1'</td>
<td>0,0,0 [0,0,0]</td>
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<td>1/2,0,0 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p_{2b.2mg}</th>
<th>Along [1,0,0] c_{p,2mm}</th>
<th>Along [0,1,0] c_{2mm}</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = -b b' = a/2</td>
<td>a' = b b' = c</td>
<td>a' = c b' = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 1/4,y,1/4</td>
</tr>
</tbody>
</table>
### Pnna'

52.5.410

### mmm'

P2'/n2, '/n2/a'

### Orthorhombic

**Origin** at \( \vec{1} \) on \( n1a' \)

**Asymmetric unit**

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2\]

**Symmetry Operations**

1. \( \mathbf{1} \)
   - \( (1 | 0,0,0) \)
2. \( \mathbf{2} \)
   - \( 1/4,0,z \)
   - \( 2 | 1/2,0,0 \)
3. \( \mathbf{2}' \)
   - \( (0,1/2,0) \)
   - \( 1/4,y,1/4 \)
   - \( 2 | 1/2,1/2,1/2 \)‘
4. \( \mathbf{2}' \)
   - \( x,1/4,1/4 \)
   - \( 2 | 0,1/2,1/2 \)‘
5. \( \mathbf{1}' \)
   - \( 0,0,0 \)
   - \( (1 | 0,0,0) \)‘
6. \( \mathbf{a}' \)
   - \( (1/2,0,0) \)
   - \( x,y,0 \)
   - \( (m_z | 1/2,0,0) \)‘
7. \( \mathbf{n} \)
   - \( (1/2,0,1/2) \)
   - \( x,1/4,z \)
   - \( (m_y | 1/2,1/2,1/2) \)
8. \( \mathbf{n} \)
   - \( (0,1/2,1/2) \)
   - \( 0,y,z \)
   - \( (m_z | 0,1/2,1/2) \)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 d 2'.</td>
<td>x,1/4,1/4 [0,v,w]</td>
</tr>
<tr>
<td>4 c .2</td>
<td>1/4,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 b 1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mg  
Along [1,0,0] c_p 2m'm'  
Along [0,1,0] c_p' 2'm'm'  

a^* = -b  b^* = a/2  
a^* = b  b^* = c  
a^* = c  b^* = a  

Origin at 0,0,z  
Origin at x,0,0  
Origin at 1/4,y,1/4
Origin at \( \bar{1} \) on \( n'1a \)

Asymmetric unit

\[
0 < x < 1; \quad 0 < y < \frac{1}{4}; \quad 0 < z < \frac{1}{2}
\]

Symmetry Operations

1. \( (1) \ 1 \quad (0,0,0) \)
2. \( (2) \ 2 \quad \frac{1}{4},0,z \quad (\frac{1}{2},1/2,0,0) \)
3. \( (3) \ 2' \quad (0,1/2,0) \quad \frac{1}{4},y,1/2 \quad (\frac{1}{2},1/2,1/2)' \)
4. \( (4) \ 2' \quad x,1/4,1/4 \quad (\frac{1}{2},0,1/2,1/2)' \)
5. \( (5) \ \bar{1} \quad 0,0,0 \quad (0,0,0) \)
6. \( (6) \ a \quad (1/2,0,0) \quad x,y,0 \quad (1/2,1/2,0,0) \)
7. \( (7) \ n' \quad (1/2,0,1/2) \quad x,1/4,z \quad (1/2,1/2,1/2)' \)
8. \( (8) \ n' \quad (0,1/2,1/2) \quad 0,y,z \quad (0,1/2,1/2)' \)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
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<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) (x + 1/2, y + 1/2, z + 1/2 ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) (x + 1/2, y + 1/2, z + 1/2 ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y + 1/2, z + 1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x + 1/2, y + 1/2, z + 1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x + 1/2, y + 1/2, z + 1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x + 1/2, y + 1/2, z + 1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x + 1/2, y + 1/2, z + 1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 d 2'..</td>
<td>x,1/4,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>(x + 1/2,3/4,1/4) [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>(x + 3/4,3/4) [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/4,3/4 [0,v,w]</td>
</tr>
<tr>
<td>4 c ..2</td>
<td>1/4,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,1/2, z + 1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
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<td>1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1] \(p_{2z} 2mg\)  
\(a^* = -b\) \(b^* = a/2\)  
Origin at 1/4,0,z  

Along [1,0,0] \(c 2' mm'\)  
\(a^* = -c\) \(b^* = b\)  
Origin at x,0,0  

Along [0,1,0] \(c 2' mm'\)  
\(a^* = -a\) \(b^* = c\)  
Origin at 1/4,y,1/4
**Origin** at $\overline{1}$ on $n1a'$

**Asymmetric unit**

$0 \leq x \leq 1$; $0 \leq y \leq 1/4$; $0 \leq z \leq 1/2$

**Symmetry Operations**

1. $\overline{1}$ $(0,0,0)$
2. $2'$ $1/4,0,z$ $(2z,1/2,0,0)'$
3. $2'$ $(0,1/2,0)$ $1/4,y,1/4$ $(2y,1/2,1/2,1/2)'$
4. $2$ $x,1/4,1/4$ $(2x,0,1/2,1/2)$
5. $\overline{1}$ $0,0,0$ $(1/2,0,0)$
6. $a'$ $(1/2,0,0)$ $x,y,0$ $(m_z,1/2,0,0)'$
7. $n'$ $(1/2,0,1/2)$ $x,1/4,z$ $(m_y,1/2,1/2,1/2)'$
8. $n$ $(0,1/2,1/2)$ $0,y,z$ $(m_z,0,1/2,1/2)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
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<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8 e 1 (1) x,y,z [u,v,w]</td>
<td>(2) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 d 2. x,1/4,1/4 [u,0,0]</td>
<td>x+1/2,3/4,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 c 2'. 1/4,0,z [u,v,0]</td>
<td>1/4,1/2, z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b 1 0,0,1/2 [u,v,w]</td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1 0,0,0 [u,v,w]</td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2'm'g  Along [1,0,0]  c_p 2' mm'  Along [0,1,0]  c 2' mm'
\(a^* = -b\)  \(b^* = a/2\)  \(a^* = b\)  \(b^* = c\)  \(a^* = -a\)  \(b^* = c\)
Origin at 0,0,z  Origin at x,0,0  Origin at 1/4,y,1/4
Origin at $\overline{1}$ on $n'1a'$

Asymmetric unit

$0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $I$

(2) $2' \cdot 1/4,0,z$

(3) $2 (0,1/2,0) \cdot 1/4,y,1/4$

(4) $2' \cdot x,1/4,1/4$

(5) $\overline{1} \cdot 0,0,0$

(6) $a' (1/2,0,0) \times y,0$

(7) $n (1/2,0,1/2) \times 1/4,z$

(8) $n' (0,1/2,1/2) \cdot 0,y,z$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

<table>
<thead>
<tr>
<th>Number</th>
<th>Symmetry</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8</td>
<td>e</td>
<td>1</td>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
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<td>(2) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(2) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
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<td>x+1/2,y,3/4,1/4 [0,v,w]</td>
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<tr>
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<td>b</td>
<td>1</td>
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<td>(11) x+1/2,y,3/4,1/4 [0,v,w]</td>
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<td>x+1/2,y,3/4,1/4 [0,v,w]</td>
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<td>a</td>
<td>1</td>
<td>x+1/2,y,3/4,1/4 [0,v,w]</td>
<td>(13) x+1/2,y,3/4,1/4 [0,v,w]</td>
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<td>x+1/2,y,3/4,1/4 [0,v,w]</td>
<td>(14) x+1/2,y,3/4,1/4 [0,v,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2'mg'  
\( a^* = -b \quad b^* = a/2 \)  
Origin at 0,0,z  
Along [1,0,0] c 2'mm'  
\( a^* = b \quad b^* = c \)  
Origin at x,0,0  
Along [0,1,0] c_p 2mm  
\( a^* = c \quad b^* = a \)  
Origin at 1/4,y,1/4
Origin at $\overline{1}^\prime$ on n'1a'

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$
   (1|0,0,0)
(2) $2$ 1/4,0,z
   (2|z|1/2,0,0)
(3) $2$ (0,1/2,0) 1/4,y,1/4
   (2|z|1/2,1/2,1/2)
(4) $2$ x,1/4,1/4
   (2|x|0,1/2,1/2)
(5) $\overline{1}$ 0,0,0
   (\overline{1}|0,0,0)'
(6) a' (1/2,0,0) x,y,0
   (m_z|1/2,0,0)'
(7) n' (1/2,0,1/2) x,1/4,z
   (m_y|1/2,1/2,1/2)'
(8) n' (0,1/2,1/2) 0,y,z
   (m_x|0,1/2,1/2)'

Pn'n'a'  m'm'm'
52.9.414  P2/n21/n2/a'
Orthorhombic
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z [u,v,w]</td>
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<tr>
<td>8 e 5</td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z [u,v,w]</td>
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</table>

| 4 d 2..      | x,1/4,1/4 [u,0,0] | x+1/2,1/4,3/4 [u,0,0] | x+3/4,3/4 [u,0,0] | x+1/2,1/4,3/4 [u,0,0] |
| 4 c .2       | 1/4,0,0 [0,0,w]   | 3/4,0,0 [0,0,w]   | 3/4,1/2,0 [0,0,w] |
| 4 b 1'       | 0,0,1/2 [0,0,0]   | 1/2,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] | 0,1/2,0 [0,0,0] |
| 4 a 1'       | 0,0,0 [0,0,0]     | 1/2,0,0 [0,0,0]   | 1/2,1/2,1/2 [0,0,0] | 0,1/2,1/2 [0,0,0] |

### Symmetry of Special Projections

- **Along [0,0,1]** p2m'g'  
  \( a^* = -b \quad b^* = a/2 \)
- **Along [1,0,0]** c2'mm'  
  \( a^* = -c \quad b^* = b \)
- **Along [0,1,0]** c2m'm'  
  \( a^* = c \quad b^* = a \)

Origin at 0,0,z  
Origin at x,0,0  
Origin at 1/4,y,1/4
Origin at center (2/m) at 2/m1

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations:

1. $1_{(1,0,0,0)}$
2. $2_{(0,0,1/2)} \cdot 1/4,0,z$
3. $2_{(1/2,0,1/2)} \cdot x,0,z$
4. $2_{x,0,0}$
5. $\overline{1}_{(0,0,0)}$
6. $a_{(1/2,0,0)} \cdot x,y,1/4$
7. $m_{(1/2,0,1/2)} \cdot x,0,z$
8. $m_{0,y,z}$

Pmna: $53.1.415$

mmm: $P2/m2/n2_1/a$

Orthorhombic
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions  
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
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<th>Position</th>
<th>Coordinates</th>
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</thead>
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<tr>
<td>8 i 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
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<tr>
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<td></td>
<td>(3) x+1/2,y,z+1/2 [u,v,w]</td>
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<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h m..</td>
<td>0,y,z [u,0,0]</td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
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<tr>
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<td></td>
<td>(7) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 g .2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
<td>(9) x+1/2,1/2,1/2 [u,0,0]</td>
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<td></td>
<td>(10) x+1/2,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 f 2..</td>
<td>x,1/2,0 [u,0,0]</td>
<td>(11) x+1/2,1/2,1/2 [u,0,0]</td>
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<tr>
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<td>(12) x+1/2,1/2,1/2 [u,0,0]</td>
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<tr>
<td>4 e 2..</td>
<td>x,0,0 [u,0,0]</td>
<td>(13) x+1/2,0,1/2 [u,0,0]</td>
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<td>(14) x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 d 2/m..</td>
<td>0,1/2,0 [u,0,0]</td>
<td>(15) x+1/2,0,1/2 [u,0,0]</td>
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<tr>
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<td>(16) x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 c 2/m..</td>
<td>1/2,1,2,0 [u,0,0]</td>
<td>(17) x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
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<td></td>
<td>(18) x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 b 2/m..</td>
<td>1/2,0,0 [u,0,0]</td>
<td>(19) x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(20) x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 a 2/m..</td>
<td>0,0,0 [u,0,0]</td>
<td>(21) x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(22) x+1/2,0,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1]  p_{2a}2m'm'
  \( a^* = a/2 \)  \( b^* = b \)
- Along [1,0,0]  p 2mg1'
  \( a^* = -c \)  \( b^* = b \)
- Along [0,1,0]  c_p 2mm'
  \( a^* = -a \)  \( b^* = c \)

Origin at 1/4,0,z  
Origin at x,0,0  
Origin at 0,y,0
Pmna1'  mmm1'  Orthorhombic
53.2.416  P2/m2/n21/a1'

Origin at center (2/m1') at 2/mn11'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

For 1 + set

(1) 1  
    (1 | 0,0,0)
    (1 | 0,0,0)

(2) 2  (0,0,1/2)  1/4,0,z  
    (2z | 1/2,0,1/2)

(3) 2'  1/4,y,1/4  
    (2z | 1/2,0,1/2)

(4) 2  x,0,0  
    (2s | 0,0,0)

(1*) 0,0,0  
    (1* | 0,0,0)

(2z* 1/2,0,1/2)  
    (2z* 1/2,0,1/2)

(3) 2  1/4,y,1/4  
    (2y | 1/2,0,1/2)

(4) 2'  x,0,0  
    (2s | 0,0,0)

(5) 1  0,0,0  
    (1 | 0,0,0)

(6) a  (1/2,0,0)  x,y,1/4  
    (mz | 1/2,0,1/2)

(7) n  (1/2,0,1/2)  x,0,z  
    (my | 1/2,0,1/2)

(8) m  0,y,z  
    (mz | 0,0,0)

(5*) 1  0,0,0  
    (1* | 0,0,0)

(6*) a' (1/2,0,0)  x,y,1/4  
    (mz | 1/2,0,1/2)

(7) n' (1/2,0,1/2)  x,0,z  
    (mz | 1/2,0,1/2)

(8) m' 0,y,z  
    (mz | 0,0,0)

For 1' + set

(1) 1'  
    (1* | 0,0,0)
    (1* | 0,0,0)

(2) 2' (0,0,1/2)  1/4,0,z  
    (2z | 1/2,0,1/2)

(3) 2'  1/4,y,1/4  
    (2y | 1/2,0,1/2)

(4) 2'  x,0,0  
    (2s | 0,0,0)

(1*) 0,0,0'  
    (1* | 0,0,0')

(2z* 1/2,0,1/2)  
    (2z* 1/2,0,1/2')

(3) 2'  1/4,y,1/4  
    (2y' | 1/2,0,1/2')

(4) 2'  x,0,0  
    (2s | 0,0,0)

(5) 1'  0,0,0  
    (1* | 0,0,0)

(6) a' (1/2,0,0)  x,y,1/4  
    (mz | 1/2,0,1/2)

(7) n' (1/2,0,1/2)  x,0,z  
    (mz' | 1/2,0,1/2')

(8) m' 0,y,z  
    (mz | 0,0,0)

(5*) 1'  0,0,0  
    (1* | 0,0,0)

(6*) a' (1/2,0,0)  x,y,1/4  
    (mz | 1/2,0,1/2)

(7) n' (1/2,0,1/2)  x,0,z  
    (mz | 1/2,0,1/2')

(8) m' 0,y,z  
    (mz | 0,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
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<td>(1) x,y,z</td>
<td>[0,0,0]</td>
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<td></td>
<td>(2) x+1/2,y,z+1/2</td>
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<tr>
<td></td>
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<td>(3) x+1/2,y,z+1/2</td>
<td>[0,0,0]</td>
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<tr>
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<td>(4) x,y,z</td>
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<td>(5) x,y,z</td>
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<td>(7) x+1/2,y,z+1/2</td>
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<td>(8) x,y,z</td>
<td>[0,0,0]</td>
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<tr>
<td>4</td>
<td>h m..1'</td>
<td>0,y,z</td>
<td>[0,0,0]</td>
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<td>1/2,y,z+1/2</td>
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<td>1/2,y,z+1/2</td>
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<td>0,y,z</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1'  Along [1,0,0] p 2mg1'  Along [0,1,0] c 2mm1'

\[a^* = a/2\]  \[b^* = b\]  \[a^* = -c\]  \[b^* = b\]  \[a^* = c\]  \[b^* = a\]

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
**Orthorhombic**

<table>
<thead>
<tr>
<th>Pm'na</th>
<th>m'mm</th>
<th>P2/m'2'/n2, 'a</th>
</tr>
</thead>
<tbody>
<tr>
<td>53.3.417</td>
<td>53.3.417</td>
<td>P2/m'2'/n2, 'a</td>
</tr>
</tbody>
</table>

**Origin** at center (2/m) at 2/m'n1

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

1. \( 1 \)
   \( (1 | 0,0,0) \)
2. \( 2' \)
   \( (0,0,1/2) \rightarrow 1/4,0,z \)
   \( (2_1 | 1/2,0,1/2)' \)
3. \( 2' \)
   \( (1/4,y,1/4) \)
   \( (2_1 | 1/2,0,1/2)' \)
4. \( 2 \)
   \( x,0,0 \)
   \( (2_1 | 0,0,0) \)
5. \( \bar{1} \)
   \( 0,0,0 \)
6. \( a \)
   \( (1/2,0,0) \rightarrow x,y,1/4 \)
   \( (m_z | 1/2,0,1/2) \)
7. \( n \)
   \( (1/2,0,1/2) \rightarrow x,0,z \)
   \( (m_y | 1/2,0,1/2) \)
8. \( m' \)
   \( 0,y,z \)
   \( (m_z | 0,0,0)' \)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w] (2) x+1/2,y,z+1/2 [u,v,w] (3) x+1/2,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w] (6) x+1/2,y,z+1/2 [u,v,w] (7) x+1/2,y,z+1/2 [u,v,w] (8) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 4 h m'..   | 0,y,z [0,v,w] 1/2,y,z+1/2 [0,v,w] 1/2,y,z+1/2 [0,v,w] 0,y,z [0,v,w] |
| 4 g .2'..  | 1/4,y,1/4 [u,0,w] 1/4,y,3/4 [u,0,w] 3/4,y,3/4 [u,0,w] 3/4,y,1/4 [u,0,w] |
| 4 f 2..    | x,1/2,0 [u,0,0] x+1/2,1/2,1/2 [u,0,0] x+1/2,1/2,1/2 [u,0,0] x+1/2,1/2,1/2 [u,0,0] |
| 4 e 2..    | x,0,0 [u,0,0] x+1/2,0,1/2 [u,0,0] x+1/2,0,1/2 [u,0,0] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_{2a}.2m'</th>
<th>Along [1,0,0]</th>
<th>p 2mg</th>
<th>Along [0,1,0]</th>
<th>c_{p}.2m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a/2</td>
<td>b* = b</td>
<td>a* = c</td>
<td>b* = a</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Orthorhombic

Pmn'a

mm'm

Orthonormic

53.4.418

P2'/m2 /n'2'/a

Origin at center (2/m) at 2'/mn'1

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2' (0,0,1/2) 1/4,0,z
(2' | 1/2,0,1/2)

(3) 2 1/4,y,1/4
(2 | 1/2,0,1/2)

(4) 2' x,0,0
(2' | 0,0,0)

(5) 1
(1 | 0,0,0)

(6) a (1/2,0,0) x,y,1/4
(m | 1/2,0,1/2)

(7) n' (1/2,0,1/2) x,0,z
(m | 1/2,0,1/2)

(8) m 0,y,z
(m | 0,0,0)
Generators selected  
(1) t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1 (1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h m.. 0,y,z [u,0,0]</td>
<td>1/2,y,z+1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,z+1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 g .2. 1/4,y,1/4 [0,v,0]</td>
<td>1/4,y,3/4 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,y,3/4 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 f 2'.. x,1/2,0 [0,v,w]</td>
<td>x+1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
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<td>x+1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 e 2'.. x,0,0 [0,v,w]</td>
<td>x+1/2,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 d 2'/m.. 0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 2'/m.. 1/2,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 2'/m.. 1/2,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 2'/m.. 0,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1], p2a-2mm
  \[ a^* = \frac{a}{2}, \quad b^* = b \]
- Along [1,0,0], p2mg1' 
  \[ a^* = -c, \quad b^* = b, \quad c^* = b \]
- Along [0,1,0], c2mm
  \[ a^* = c, \quad b^* = a \]
Pmna'  Orthorhombic  53.5.419

mmm'  P2'/m2'/n21/a'

Origin at center (2'/m) at 2'/mn1

Asymmetric unit  0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1;  0 ≤ z ≤ 1/4

Symmetry Operations

(1)  1  (1 | 0,0,0)
(2)  2  (0,0,1/2)  1/4,0,z  (2 | 1/2,0,1/2)
(3)  2'  1/4,y,1/4  (2 | 1/2,0,1/2)'
(4)  2'  x,0,0  (2 | 0,0,0)'
(5)  1'  0,0,0  (1 | 0,0,0)'
(6)  a' (1/2,0,0)  x,y,1/4  (m | 1/2,0,1/2)'
(7)  n (1/2,0,1/2)  x,0,z  (m | 1/2,0,1/2)
(8)  m  0,y,z  (m | 0,0,0)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 h m..</td>
<td>0,y,z [u,0,0]</td>
<td>1/2,y,z+1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 g ..2'.</td>
<td>1/4,y,1/4 [u,0,w]</td>
<td>1/4,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>4 f 2'.</td>
<td>x,1/2,0 [0,v,w]</td>
<td>x+1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 e 2'.</td>
<td>x,0,0 [0,v,w]</td>
<td>x+1/2,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 d 2'/m..</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 2'/m..</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 2'/m..</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 2'/m..</td>
<td>0,0,0 [0,0,0]</td>
<td>2/0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p2mm</td>
<td>a* = a/2</td>
<td>p 2mg1'</td>
<td>c_p 2mm</td>
</tr>
<tr>
<td>b* = b</td>
<td>a* = -c</td>
<td>a* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (2'/m') at 2'/m'n'1

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations:

1. (1) 1
   (1) 0,0,0

2. (2) 2 (0,0,1/2) 1/4,0,z
   (2) 1/2,0,1/2)

3. (3) 2' 1/4,y,1/4
   (2') 1/2,0,1/2)

4. (4) 2' x,0,0
   (2') 0,0,0)

5. (5) (0,0,0)
   (1) 0,0,0

6. (6) a (1/2,0,0) x,y,1/4
   (m_x 1/2,0,1/2)

7. (7) n' (1/2,0,1/2) x,0,z
   (m_y 1/2,0,1/2)

8. (8) m' 0,y,z
   (m_z 0,0,0)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
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<tbody>
<tr>
<td>8 i 1 (1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 h m'.. 0,y,z [0,v,w]</td>
<td>1/2,y,z+1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 g .2'.. 1/4,y,1/4 [u,0,w]</td>
<td>1/4,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>4 f 2'.. x,1/2,0 [0,v,w]</td>
<td>x+1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 e 2'.. x,0,0 [0,v,w]</td>
<td>x+1/2,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 d 2/m'.. 0,1/2,0 [0,v,w]</td>
<td>1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 c 2/m'.. 1/2,1/2,0 [0,v,w]</td>
<td>0,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 b 2/m'.. 1/2,0,0 [0,v,w]</td>
<td>0,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 a 2/m'.. 0,0,0 [0,v,w]</td>
<td>1/2,0,1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2m'2m'  
  a* = a/2  b* = b  
  Origin at 0,0,z
- Along [1,0,0] p 2'mg'  
  a* = -c  b* = b  
  Origin at x,0,0
- Along [0,1,0] c2' 2mm'  
  a* = c  b* = a  
  Origin at 0,y,0
Origin at center \((2/m)\) at \(2/mn'1\)

Asymmetric unit \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/4\)

Symmetry Operations

(1) \(\overline{1}\ (1\ |0,0,0)\)

(2) \(2' (0,0,1/2) \ 1/4,0,z\)

(3) \(2' 1/4,y,1/4\)

(4) \(2 \ x,0,0\)

(5) \(\overline{1} \ 0,0,0\)

(6) \(a' (1/2,0,0) \ x,y,1/4\)

(7) \(n' (1/2,0,1/2) \ x,0,z\)

(8) \(m \ 0,y,z\)

Pmn'a'\ 53.7.421

mm'm'\ P2/m2' /n'2, /a'

Orthorhombic
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w] (3) x+1/2,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 h m..</td>
<td>0,y,z [u,0,0]</td>
<td>1/2,y,z+1/2 [u,0,0] 1/2,y,z+1/2 [u,0,0] 0,y,z [u,0,0]</td>
</tr>
<tr>
<td>4 g .2'</td>
<td>1/4,y,1/4 [u,0,w]</td>
<td>1/4,y,3/4 [u,0,w] 3/4,y,3/4 [u,0,w] 3/4,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 f 2..</td>
<td>x,1/2,0 [u,0,0]</td>
<td>x+1/2,1/2,1/2 [u,0,0] x+1/2,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 e 2..</td>
<td>x,0,0 [u,0,0]</td>
<td>x+1/2,0,1/2 [u,0,0] x+1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 d 2/m..</td>
<td>0,1/2,0 [u,0,0]</td>
<td>1/2,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 c 2/m..</td>
<td>1/2,1/2,0 [u,0,0]</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 b 2/m..</td>
<td>1/2,0,0 [u,0,0]</td>
<td>0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 a 2/m..</td>
<td>0,0,0 [u,0,0]</td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm'  
  \[ a'^* = a/2 \quad b'^* = b \]
- Along [1,0,0] p 2mg1'  
  \[ a'^* = -c \quad b'^* = b \]
- Along [0,1,0] c 2mm'  
  \[ a'^* = -a \quad b'^* = c \]

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center (2'/m') at 2'/m'n1

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1 (1 0 0 0)
(2) 2' (0,0,1/2) 1/4,0,z
   (2' 1/2,0,1/2)
(5) 1 -0,0,0 (1 0 0 0)
(6) a' (1/2,0,0) x,y,1/4
    (m_z 1/2,0,1/2)
(7) n (1/2,0,1/2) x,0,z
    (m_y 1/2,0,1/2)
(8) m' 0,y,z (m_z 0,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 h m'..</td>
<td>0,y,z [0,v,w]</td>
<td>1/2,y,z+1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 g .2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
<td>1/4,y,3/4 [0,v,0]</td>
</tr>
<tr>
<td>4 f .2'..</td>
<td>x,1/2,0 [0,v,w]</td>
<td>x+1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 e .2'..</td>
<td>x,0,0 [0,v,w]</td>
<td>x+1/2,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 d .2'/m'..</td>
<td>0,1/2,0 [0,v,w]</td>
<td>1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 c .2'/m'..</td>
<td>1/2,1/2,0 [0,v,w]</td>
<td>0,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 b .2'/m'..</td>
<td>1/2,0,0 [0,v,w]</td>
<td>0,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>2 a .2'/m'..</td>
<td>0,0,0 [0,v,w]</td>
<td>1/2,0,1/2 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin</th>
<th>Along [0,0,1] p2mm'</th>
<th>Along [1,0,0] p 2'm'g</th>
<th>Along [0,1,0] c_p 2'2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = -b b^* = a/2</td>
<td>a^* = -c b^* = b</td>
<td>a^* = c b^* = a</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at center (2/m') at 2/m'n'1

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

<table>
<thead>
<tr>
<th>Symmetry Operations</th>
<th>( (1,0,0) )</th>
<th>( (0,0,1/2) )</th>
<th>( 1/4,0,z )</th>
<th>( x,0,0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1 )</td>
<td>( 2 )</td>
<td>( 3 )</td>
<td>( 4 )</td>
<td>( 5 )</td>
</tr>
<tr>
<td>( 1 )</td>
<td>( 2 )</td>
<td>( 3 )</td>
<td>( 4 )</td>
<td>( 5 )</td>
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<td>( 1 )</td>
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<td>( 3 )</td>
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<td>( 5 )</td>
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<tr>
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<td>( 5 )</td>
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<table>
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<tr>
<th>Symmetry Operations</th>
<th>( (1/2,0,0) )</th>
<th>( x,y,1/4 )</th>
<th>( x,0,z )</th>
<th>( 0,y,z )</th>
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<tr>
<td>( 6 )</td>
<td>( 7 )</td>
<td>( 8 )</td>
<td>( 6' )</td>
<td>( 7' )</td>
</tr>
<tr>
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<td>( 7 )</td>
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<td>( 7 )</td>
<td>( 8 )</td>
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<td>( 7' )</td>
</tr>
</tbody>
</table>
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,   Coordinates
Wyckoff letter, Site Symmetry.

8  i  1 (1) x,y,z [u,v,w] (2) x+1/2,y,z+1/2 [u,v,w] (3) x+1/2,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w] (6) x+1/2,y,z+1/2 [u,v,w] (7) x+1/2,y,z+1/2 [u,v,w] (8) x,y,z [u,v,w]

4  h  m'.. 0,y,z [0,v,w] 1/2,y,z+1/2 [0,v,w] 1/2,y,z+1/2 [0,v,w] 0,y,z [0,v,w]

4  g  .2. 1/4,y,1/4 [0,v,0] 1/4,y,3/4 [0,v,0] 3/4,y,3/4 [0,v,0] 3/4,y,1/4 [0,v,0]

4  f  2.. x,1/2,0 [u,0,0] x+1/2,1/2,1/2 [u,0,0] x,1/2,0 [u,0,0] x+1/2,1/2,1/2 [u,0,0]

4  e  2.. x,0,0 [u,0,0] x+1/2,0,1/2 [u,0,0] x,0,0 [u,0,0] x+1/2,0,1/2 [u,0,0]

2  d  2/m'.. 0,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]

2  c  2/m'.. 1/2,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0]

2  b  2/m'.. 1/2,0,0 [0,0,0] 0,0,1/2 [0,0,0]

2  a  2/m'.. 0,0,0 [0,0,0] 1/2,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2m'm' Along [1,0,0] p 2m'g' Along [0,1,0] c 2m'm'

\( a^* = a/2 \) \( b^* = b \) \( a^* = -c \) \( b^* = b \)

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at center (2/m) at 2/mn1

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

1. 1
   0,0,0

2. 2 (0,0,1/2) 1/4,0,z
   2 | 1/2,0,1/2

3. 2 1/4,y,1/4
   2 | 1/2,0,1/2

4. 2 x,0,0
   2 | 0,0,0

5. m 0,0,0
   m | 1/2,0,1/2

6. a (1/2,0,0) x,y,1/4
   m | 1/2,0,1/2

7. n (1/2,0,1/2) x,0,z
   n | 1/2,0,1/2

8. m 0,y,z
   m | 0,0,0

For (0,1,0)' + set

1. t' (0,1,0)
   0,1,0'

2. 2' (0,0,1/2) 1/4,1/2,z
   2 | 1/2,1,1/2'

3. 2' (0,1,0) 1/4,y,1/4
   2 | 1/2,1,1/2'

4. 2' x,1/2,0
   2 | 0,1,0'

5. t' 0,1/2,0
   0,1,0'

6. n' (1/2,1,0) x,y,1/4
   m | 1/2,1,1/2'

7. n' (1/2,0,1/2) x,1/2,z
   m | 1/2,1,1/2'

8. b' (0,1,0) 0,y,z
   m | 0,1,0'

Orthonormic

P₂b mna
53.10.424

mmm1'
P₂b 2/m2/n21/a
Generators selected  (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<th>Coordinates</th>
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<tr>
<td>(0,0,0)</td>
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<td>(0,1,0)</td>
<td>(0,1,0) +</td>
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<tr>
<td>16</td>
<td></td>
<td>8</td>
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</tr>
<tr>
<td>i</td>
<td>1</td>
<td>h</td>
<td>m..</td>
</tr>
<tr>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
<td>0,y,z [u,0,0]</td>
<td>1/2,y,z+1/2 [u,0,0]</td>
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<tr>
<td>8</td>
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<td>g</td>
<td>.2.</td>
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<tr>
<td>x,1/2,0 [0,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
<td>1/4,y,1/4 [0,v,0]</td>
<td>1/4,y,3/4 [0,v,0]</td>
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<tr>
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<td></td>
<td>f</td>
<td>2'.</td>
</tr>
<tr>
<td>x,0,0 [u,0,0]</td>
<td>(3) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>e</td>
<td>2..</td>
</tr>
<tr>
<td>x,0,0 [u,0,0]</td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
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<tr>
<td>4</td>
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<td>c</td>
<td>2/m.</td>
</tr>
<tr>
<td>0,1/2,0 [0,0,0]</td>
<td>(8) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(8) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(8) x+1/2,y,z+1/2 [u,v,w]</td>
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<tr>
<td>4</td>
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<td>b</td>
<td>2/m.</td>
</tr>
<tr>
<td>0,0,0 [u,0,0]</td>
<td>(9) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(9) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(9) x+1/2,y,z+1/2 [u,v,w]</td>
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<td>a</td>
<td>2/m.</td>
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<tr>
<td>0,0,0 [u,0,0]</td>
<td>(10) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(10) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(10) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p c 2mm  
Along [1,0,0]  p 2mg 1'  
Along [0,1,0]  c 2mm 1'  

a' = a/2  
b' = b  
a' = -c  
b' = b  
a' = c  
b' = a  
Origin at 0,1/2,z  
Origin at x,0,0  
Origin at 0,y,0
Orthorhombic

Origin at center (2/m') at 2/m'n1

Asymmetric unit

0 < x < 1/2; 0 < y < 1; 0 < z < 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1 | 0,0,0)

(5) T' 0,0,0
    (1 | 0,0,0)

(2) 2' (0,0,1/2) 1/4,0,z
    (2_ | 1/2,0,1/2)

(6) a (1/2,0,0) x,y,1/4
    (m_ | 1/2,0,1/2)

(7) n (1/2,0,1/2) x,0,z
    (m_ | 1/2,0,1/2)

(8) m' 0,y,z
    (m_ | 0,0,0)

For (0,1,0) + set

(1) t' (0,1,0)
    (1 | 0,1,0)

(5) T 0,1/2,0
    (1 | 0,1,0)

(2) 2 (0,0,1/2) 1/4,1/2,z
    (2_ | 1/2,1,1/2)

(6) n' (1/2,1,0) x,y,1/4
    (m_ | 1/2,1,1/2)

(7) n' (1/2,0,1/2) x,1/2,z
    (m_ | 1/2,1,1/2)

(8) b (0,1,0) 0,y,z
    (m_ | 0,1,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>(0,1,0)'+</td>
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<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
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<td>(3) x+1/2,y,z+1/2 [u,v,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<td>8 h m'..</td>
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<td>1/4,y,1/4 [0,v,0]</td>
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<td>1/2,y,z+1/2 [0,v,w]</td>
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<td>x+1/2,0,1/2 [u,0,0]</td>
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<td>0,1/2,0 [0,v,w]</td>
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<td>4 a 2/m'..</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p c2mm  Along [1,0,0]  p 2bc 2mg  Along [0,1,0]  c2mm1'
a* = a/2   b* = b   a* = -c   b* = b   a* = c   b* = a
Origin at 1/4,1/2,z  Origin at x,0,0  Origin at 0,y,0
Origin at center (2/m) at 2/mn1

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1 | 0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z  
(2z | 1/2,0,1/2)

(3) 2′ 1/4,y,1/4  
(2z | 1/2,0,1/2)′

(4) 2′ x,0,0  
(2z | 0,0,0)′

(5) 1′ 0,0,0  
(1 | 0,0,0)′

(6) a′ (1/2,0,0) x,y,1/4  
(m2 | 1/2,0,1/2)′

(7) n (1/2,0,1/2) x,0,z  
(m2 | 1/2,0,1/2)

(8) m 0,y,z  
(m2 | 0,0,0)

For (0,1,0)′ + set

(1) t′ (0,1,0)  
(1 | 0,1,0)′

(2) 2′ (0,0,1/2) 1/4,1/2,z  
(2z | 1/2,1,1/2)′

(3) 2 (0,1,0) 1/4,y,1/4  
(2z | 1/2,1,1/2)

(4) 2 x,1/2,0  
(2z | 0,1,0)

(5) 1′ 0,1/2,0  
(1 | 0,1,0)

(6) n (1/2,1,0) x,y,1/4  
(m2 | 1/2,1,1/2)

(7) n′ (1/2,0,1/2) x,1/2,z  
(m2 | 1/2,1,1/2)′

(8) b′ (0,1,0) 0,y,z  
(m2 | 0,1,0)′
Generators selected (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<tr>
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<td>(0,1,0)' +</td>
</tr>
<tr>
<td>16 i</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2, y, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x, y, z [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x, y, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2, y, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2, y, z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(8) x, y, z [u,v,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>1/4,y,1/4 [u,0,w]</td>
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<tr>
<td>8 f</td>
<td>x,1/2,0 [u,0,0]</td>
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<tr>
<td>8 e</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>4 d</td>
<td>0,1/2,0 [u,0,0]</td>
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<tr>
<td>4 c</td>
<td>1/2,1/2,0 [u,0,0]</td>
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<tr>
<td>4 b</td>
<td>1/2,0,0 [0,0,0]</td>
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<tr>
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<td>0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] P_{2b}2mm Along [1,0,0] p 2mg1' Along [0,1,0] c 2mm1'

\( a^* = -b \) \( b^* = a/2 \)

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at center (2'/m') at 2'/m'n1

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

1. 1 (0,0,0)
2. 2' (0,0,1/2) 1/4,0,z
3. 2 1/4,1/2,z
4. 2' x,0,0

For (0,1,0)' + set

1. t' (1,0,0)
2. 2 (1,0,1/2) 1/4,1/2,z
3. 2' (0,1,0) 1/4,y,1/4
4. 2 x,1/2,0

For (0,0,1) + set

1. t' (1,0,0)
2. 2 (0,0,1/2) 1/4,1/2,z
3. 2' (0,0,1/2) 1/4,y,1/4
4. 2 x,1/2,0

For (0,1,0)' + set

1. t' (1,0,0)
2. 2 (1,0,1/2) 1/4,1/2,z
3. 2' (0,1,0) 1/4,y,1/4
4. 2 x,1/2,0

For (0,1,0) + set

1. t' (1,0,0)
2. 2 (0,0,1/2) 1/4,1/2,z
3. 2' (0,1,0) 1/4,y,1/4
4. 2 x,1/2,0

53.13.427 - 1 - 844
Generators selected  (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(0,1,0)’ +</td>
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<tr>
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<td>(2) x+1/2,y,z+1/2 [u,v,w] (3) x+1/2,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w]</td>
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<td>1/2,y,z+1/2 [0,v,w] 1/2,y,z+1/2 [0,v,w] 0,y,z [0,v,w]</td>
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<tr>
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<tr>
<td>4 b 2/m’ .. 1/2,0,0 [0,v,w]</td>
<td>0,0,1/2 [0,v,w]</td>
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<tr>
<td>4 a 2/m’ .. 0,0,0 [0,v,w]</td>
<td>1/2,0,1/2 [0,v,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a-2m’m’  Along [1,0,0] p2a-2m’g’  Along [0,1,0] c2mm1’
a* = -b  b* = a/2  a* = -c  b* = b  a* = c  b* = a
Origin at 0,1/2,z  Origin at x,1/4,0  Origin at 0,y,0
Pcca  
54.1.428  
Orthorhombic

mmm  
P2₁/c2/c2/a

Origin at 1 on 1ca

Asymmetric unit  
0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1  
(1 | 0,0,0)

(2) 2  
1/4,0,z  
(2 | 1/2,0,0)

(3) 2  
0,y,1/4  
(2 | 0,0,1/2)

(4) 2  
(1/2,0,0)  
x,0,1/4  
(2 | 1/2,0,1/2)

(5) 1  
0,0,0  
(1 | 0,0,0)

(6) a  
(1/2,0,0)  
x,y,0  
(m₂ | 1/2,0,0)

(7) c  
(0,0,1/2)  
x,0,z  
(m_y | 0,0,1/2)

(8) c  
(0,0,1/2)  
1/4,y,z  
(m_z | 1/2,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2, y,v [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2, y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,v, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2, y,v [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2, y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 e ..2</td>
<td>3/4,1/2, z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2, z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 d ..2</td>
<td>3/4,0, z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,0, z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 c ..2</td>
<td>0,y,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [0,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p2a.2mm</td>
<td>a^* = a/2  b^* = b</td>
</tr>
<tr>
<td></td>
<td>Origin at 1/4,0,z</td>
</tr>
<tr>
<td>Along [1,0,0] p2a.2m'm'</td>
<td>a^* = -c/2  b^* = b</td>
</tr>
<tr>
<td></td>
<td>Origin at x,1/2,0</td>
</tr>
<tr>
<td>Along [0,1,0] p2b.2m'g'</td>
<td>a^* = -a  b^* = c/2</td>
</tr>
<tr>
<td></td>
<td>Origin at 0,y,1/4</td>
</tr>
</tbody>
</table>
Origin at \( \bar{1}' \) on 1ca1'

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

For 1 + set

1. \( 1 \) 0,0,0
   (1) 1
   (2) \( 2 \) 1/4,0,z
   (3) \( 2' \) 0,y,1/4
   (4) \( 2' (1/2,0,0) \) x,0,1/4

2. \( 0,0,0 \)
   (5) \( \bar{1} \) 0,0,0
   (6) a (1/2,0,0) x,y,0
   (7) c (0,0,1/2) x,0,z
   (8) c (0,0,1/2) 1/4,y,z

3. \( \bar{1} \) 0,0,0
   (5) \( \bar{1} \) 0,0,0
   (6) a' (1/2,0,0) x,y,0
   (7) c' (0,0,1/2) x,0,z
   (8) c' (0,0,1/2) 1/4,y,z

For 1' + set

1. \( 1' \) 0,0,0
   (1) 1' 0,0,0
   (2) \( 2' \) 1/4,0,z
   (3) \( 2' \) 0,y,1/4
   (4) \( 2' (1/2,0,0) \) x,0,1/4

2. \( 0,0,0 \)
   (5) \( \bar{1} \) 0,0,0
   (6) a (1/2,0,0) x,y,0
   (7) c (0,0,1/2) x,0,z
   (8) c (0,0,1/2) 1/4,y,z

3. \( \bar{1} \) 0,0,0'
   (5) \( \bar{1} \) 0,0,0'
   (6) a' (1/2,0,0) x,y,0
   (7) c' (0,0,1/2) x,0,z
   (8) c' (0,0,1/2) 1/4,y,z
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 +</td>
</tr>
<tr>
<td>8 f 11' (1) x,y,z [0,0,0]</td>
<td>(2) (\bar{x}+1/2,\bar{y},z) [0,0,0]</td>
</tr>
<tr>
<td>(5) (x,y,\bar{z}) [0,0,0]</td>
<td>(6) (x+1/2,y,z) [0,0,0]</td>
</tr>
<tr>
<td>4 e ..21' 1/4,1/2,z [0,0,0]</td>
<td>3/4,1/2,(\bar{z}+1/2) [0,0,0]</td>
</tr>
<tr>
<td>4 d ..21' 1/4,0,z [0,0,0]</td>
<td>3/4,0,(\bar{z}+1/2) [0,0,0]</td>
</tr>
<tr>
<td>4 c .2.1' 0,y,1/4 [0,0,0]</td>
<td>1/2,(\bar{y},1/4) [0,0,0]</td>
</tr>
<tr>
<td>4 b (\bar{1}) 1' 0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a (\bar{1}) 1' 0,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2mm1'</th>
<th>Along [1,0,0] p2mm1'</th>
<th>Along [0,1,0] p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a/2) b* = b</td>
<td>(a^* = b) b* = c/2</td>
<td>(a^* = -a) b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
54.3.430 - 1 - 850

Pc'ca

54.3.430

m'mm

P2_1/c'2'/c2'/a

Orthorhombic

Origin at \( \bar{1} \) on 1ca

Asymmetric unit

\( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) \( 2' \)
\( 1/4,0,z \)
\( \bar{2}_z \bar{1}/2,0,0' \)

(3) \( 2' \)
\( 0,y,1/4 \)
\( \bar{2}_y 0,0,1/2' \)

(4) \( 2 \)
\( (1/2,0,0) \)
\( x,y,0 \)

(5) \( 1 \)
\( 0,0,0 \)
\( (1 | 0,0,0)' \)

(6) \( a \)
\( (1/2,0,0) \)
\( x,y,0 \)
\( \bar{m}_z 1/2,0,0 \)

(7) \( c \)
\( (0,0,1/2) \)
\( x,0,z \)
\( \bar{m}_y 0,0,1/2 \)

(8) \( c' \)
\( (0,0,1/2) \)
\( 1/4,y,z \)
\( \bar{m}_z 1/2,0,1/2' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x +1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 e .2'</td>
<td>1/4,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/4,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 d .2'</td>
<td>1/4,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/4,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>4 b .1'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a .1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mm'

<table>
<thead>
<tr>
<th>a'</th>
<th>b'</th>
</tr>
</thead>
<tbody>
<tr>
<td>-b</td>
<td>a/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Along [1,0,0] p 2mm

<table>
<thead>
<tr>
<th>a'</th>
<th>b'</th>
</tr>
</thead>
<tbody>
<tr>
<td>b</td>
<td>c/2</td>
</tr>
</tbody>
</table>

Origin at x,0,0

Along [0,1,0] p2b, 2mg

<table>
<thead>
<tr>
<th>a'</th>
<th>b'</th>
</tr>
</thead>
<tbody>
<tr>
<td>-a</td>
<td>c/2</td>
</tr>
</tbody>
</table>

Origin at 0,y,0
**Pcc'a**

54.4.431

Orthorhombic

**mm'm**

P2₁/c2/c'2'/a

*Origin* at 1 on 1c'a

*Asymmetric unit* 

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

*Symmetry Operations*

1. \( (1) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \)

2. \( (2) \begin{pmatrix} 1/4 \\ 0 \\ z \end{pmatrix} \)

3. \( (3) \begin{pmatrix} 0 \\ y, 1/4 \end{pmatrix} \)

4. \( (4) \begin{pmatrix} 1/2, 0, 0 \end{pmatrix} \)

5. \( (5) \begin{pmatrix} 0, 0, 0 \end{pmatrix} \)

6. \( (6) \begin{pmatrix} 1/2, 0, 0 \end{pmatrix} \)

7. \( (7) \begin{pmatrix} 0, 0, 1/2 \end{pmatrix} \)

8. \( (8) \begin{pmatrix} 0, 0, 1/2 \end{pmatrix} \)

Diagram:

- **Pcc'a**
- **mm'm**
- Orthorhombic structure with symmetry elements indicated.
Continued

Generators selected
(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Positions

Coordinates

8 f 1 (1) x,y,z [u,v,w] (2) x+1/2,y,z [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x+1/2,y,z+1/2 [u,v,w] (5) x,y,z [u,v,w] (6) x+1/2,y,z [u,v,w] (7) x,y,z+1/2 [u,v,w] (8) x+1/2,y,z+1/2 [u,v,w]

4 e .2' 1/4,1/2,z [u,v,0] 3/4,1/2,z [u,v,0] 3/4,1/2,z [u,v,0] 1/4,1/2,z+1/2 [u,v,0]

4 d .2' 1/4,0,z [u,v,0] 3/4,0,z [u,v,0] 3/4,0,z [u,v,0] 1/4,0,z+1/2 [u,v,0]

4 c .2 0,y,1/4 [0,v,0] 1/2,y,1/4 [0,v,0] 0,y,3/4 [0,v,0] 1/2,y,3/4 [0,v,0]

4 b .1' 0,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]

4 a .1' 0,0,0 [0,0,0] 1/2,0,0 [0,0,0] 0,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] $p_{2a'2m'm'}$

Along [1,0,0] $p_{2a'2mm}$

Along [0,1,0] $p_{2b'2m'g'}$

$a^* = a/2$ $b^* = b$

$a^* = -c/2$ $b^* = b$

$a^* = -a$ $b^* = c/2$

Origin at 0,0,z

Origin at x,0,0

Origin at 0,y,0
**Orthorhombic**

### Pcca'

- **Symmetry Operations**

1. $1$
   
   $[1 | 0,0,0]$

2. $2$
   
   $1/4,0,z$
   
   $[2 | 1/2,0,0]$

3. $2'$
   
   $0,y,1/4$
   
   $[2 | 0,0,1/2]'$

4. $2'(1/2,0,0)$
   
   $x,0,1/4$
   
   $[2 | 1/2,0,1/2]'$

5. $1'$
   
   $0,0,0$

6. $a'(1/2,0,0)$
   
   $x,y,0$
   
   $[m | 1/2,0,0]'$

7. $c(0,0,1/2)$
   
   $x,0,z$
   
   $[m | 0,0,1/2]$

8. $c(0,0,1/2)$
   
   $1/4,y,z$
   
   $[m | 1/2,0,1/2]$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Origin** at $1'$ on 1ca'

---

**mmm'**

- **Symmetry Operations**

### P₂₁'/c₂'/c₂/a'

1. $1$
   
   $[1 | 0,0,0]$

2. $2$
   
   $1/4,0,z$
   
   $[2 | 1/2,0,0]$

3. $2'$
   
   $0,y,1/4$
   
   $[2 | 0,0,1/2]'$

4. $2'(1/2,0,0)$
   
   $x,0,1/4$
   
   $[2 | 1/2,0,1/2]'$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Origin** at $1'$ on 1ca'
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1 (1) x,y,z [u,v,w] (2) x+1/2,y,z [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x+1/2,y,z+1/2 [u,v,w] (5) x,y,z [u,v,w] (6) x+1/2,y,z [u,v,w] (7) x,y,z+1/2 [u,v,w] (8) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 e .2 1/4,1/2,z [0,0,w] 3/4,1/2,z+1/2 [0,0,w] 3/4,1/2,z [0,0,w] 1/4,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 d .2 1/4,0,z [0,0,w] 3/4,0,z+1/2 [0,0,w] 3/4,0,z [0,0,w] 1/4,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 c .2' 0,y,1/4 [u,0,w] 1/2,y,1/4 [u,0,w] 0,y,3/4 [u,0,w] 1/2,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>4 b 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1/2,0,0 [0,0,0] 1/2,0,0 [0,0,0] 1/2,0,0 [0,0,0] 1/2,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**  p2mm  
  
  - **Along [1,0,0]**  p2a' 2m'm'  
    - a^* = a/2  b^* = b  
    - a^* = -c/2  b^* = b  
  
  - **Along [0,1,0]**  p2b' 2m'g'  
    - a^* = -a  b^* = c/2  
    - Origin at x,0,0  
    - Origin at 0,0,z  
    - Origin at 0,y,0
**Origin** at $\overline{1}$ on 1c'a

**Asymmetric unit**

\[0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad T' \quad 0,0,0 \\
(2) & \quad 2 \quad \frac{1}{4},0,z \\
(3) & \quad 2' \quad 0,y,1/4 \\
(4) & \quad 2' \quad \frac{1}{2},0,0 \\
(5) & \quad \overline{1} \quad 0,0,0 \\
(6) & \quad a \quad \frac{1}{2},0,0 \\
(7) & \quad c' \quad 0,0,1/2 \\
(8) & \quad c' \quad 0,0,1/2 \\
\end{align*}
\]

---

**Pc"c'a**

<table>
<thead>
<tr>
<th>Symmetry Type</th>
<th>Space Group</th>
<th>Number</th>
<th>Symbols</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orthorhombic</td>
<td>P2, 2/c'2/c'2/a</td>
<td>54.6.433</td>
<td>Pc&quot;c'a</td>
</tr>
</tbody>
</table>

---

**m'\text{m}'m**
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) ( \bar{x} + 1/2, \bar{y}, z ) [u,v,w]</td>
<td>(3) ( \bar{x}, \bar{y}, \bar{z} + 1/2 ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) ( x + 1/2, \bar{y}, \bar{z} + 1/2 ) [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) ( \bar{x}, \bar{y}, \bar{z} ) [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 e ..2</td>
<td>1/4,1/2,z [0,0,w]</td>
<td>3/4,1/2,( z + 1/2 ) [0,0,w]</td>
<td>3/4,1/2,( \bar{z} ) [0,0,w]</td>
</tr>
<tr>
<td>4 d ..2</td>
<td>1/4,0,z [0,0,w]</td>
<td>3/4,0,( \bar{z} + 1/2 ) [0,0,w]</td>
<td>3/4,0,( z ) [0,0,w]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td>1/2,( \bar{y}, 1/4 ) [u,0,w]</td>
<td>0,( \bar{y}, 3/4 ) [u,0,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>1/2,1/2,0 [u,v,w]</td>
<td>1/2,1/2,( \bar{u}, \bar{v}, w )</td>
<td>0,( \bar{u}, \bar{v}, w )</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
<td>1/2,0,0 [( u, v ),w]</td>
<td>0,0,1/2 [( u, v ),w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,0,1/2 [( u, v ),w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p 2( m )m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a/2 ) ( b^* = b )</td>
<td>( a^* = -c/2 ) ( b^* = b )</td>
</tr>
<tr>
<td>Origin at 1/4,0,z</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>

54.6.433 - 2 - 857
Pcc'a'  
54.7.434

mm'm'  
P2_1/c2'/c'2'/a'

Orthorhombic

Origin at 1 on 1c'a'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1  
(1|0,0,0)  
(5) 1  
(1|0,0,0)

(2) 2' 1/4,0,z  
(2_z|1/2,0,0)'  
(6) a' (1/2,0,0)  
(m_z|1/2,0,0)'

(3) 2' 0,y,1/4  
(2|0,0,1/2)'  
(7) c' (0,0,1/2)  
(m_y|0,0,1/2)'

(4) 2 (1/2,0,0)  
x,0,1/4  
(2|1/2,0,1/2)

54.7.434 - 1 - 858
Continued

54.7.434 Pcc'a'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x, y, z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>4 e .2'</td>
<td>1/4,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 d .2'</td>
<td>1/4,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mm'  Along [1,0,0] p2a*2mm  Along [0,1,0] p 2'mg'  
\(a^* = a/2\)  \(b^* = b\)  \(a^* = -a\)  \(b^* = c/2\)
Origin at 1 on 1ca'

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

1. (1) 1 (0,0,0,0)
   (1,0,0,0)
2. (2) 2' 1/4,0,z (2,1/2,0,0)
   (2,1/2,0,0)
3. (3) 2 0,y,1/4 (2,0,0,1/2)
   (2,0,0,1/2)
4. (4) 2' (1/2,0,0) x,0,1/4 (2,1/2,0,1/2)
   (2,1/2,0,1/2)
5. (5) 1 0,0,0 (1,0,0,0)
   (1,0,0,0)
6. (6) a' (1/2,0,0) x,y,0 (m_z,1/2,0,0)
   (m_z,1/2,0,0)
7. (7) c (0,0,1/2) x,0,z (m_y,0,1/2)
   (m_y,0,1/2)
8. (8) c' (0,0,1/2) 1/4,y,z (m_z,1/2,0,1/2)
   (m_z,1/2,0,1/2)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
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<tr>
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<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) ( x+1/2, y, z ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) ( x, y, z+1/2 ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) ( x+1/2, y, z+1/2 ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) ( x, y, z ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) ( x+1/2, y, z ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) ( x, y, z+1/2 ) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) ( x+1/2, y, z+1/2 ) [u,v,w]</td>
</tr>
<tr>
<td>4 e .2'</td>
<td>1/4,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,( z+1/2 ) [u,v,0]</td>
</tr>
<tr>
<td>4 d .2'</td>
<td>1/4,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,0,( z+1/2 ) [u,v,0]</td>
</tr>
<tr>
<td>4 c .2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>( 1/2, y ,1/4 ) [0,v,0]</td>
</tr>
<tr>
<td>4 b ( \bar{1} )</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>( 1/2, 1/2, 0 ) [u,v,w]</td>
</tr>
<tr>
<td>4 a ( \bar{1} )</td>
<td>0,0,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>( 1/2,0,0 ) [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'mm' Along [1,0,0] p 2'mm' Along [0,1,0] p_{21v} 2m'g'

\( a^* = -b \) \( b^* = a/2 \) \( a^* = b \) \( b^* = c/2 \) \( a^* = -a \) \( b^* = c/2 \)

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
**Origin** at \( \bar{1} \) on 1c'a'

**Asymmetric unit**
\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2
\]

**Symmetry Operations**

1. \( 1 \) (1) 1
   - (1) (0,0,0)
2. \( 2 \) (2) \( 1/4,0,z \)
   - (2) (0,0,1/4)
3. \( 2 \) (3) \( 0,y,1/4 \)
   - (3) (0,0,1/2)
4. \( 2 \) (4) \( (1/2,0,0) x,0,1/4 \)
   - (4) \( (1/2,0,1/2) \)
5. \( \bar{1} \) (5) \( 0,0,0 \)
   - (5) (0,0,0)'
6. \( a' \) (6) \( (1/2,0,0) x,y,0 \)
   - (6) \( (1/2,0,0) \)
7. \( c' \) (7) \( (0,0,1/2) x,0,z \)
   - (7) \( (0,0,1/2) \)
8. \( c' \) (8) \( (0,0,1/2) 1/4,y,z \)
   - (8) \( (0,0,1/2) \)
Continued

54.9.436

Pc'c'a'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 e ..2</td>
<td>1/4,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 d ..2</td>
<td>1/4,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 c .2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'   Along [1,0,0] p 2'm'm'   Along [0,1,0] p 2m'g'

a* = a/2  b* = b      a* = -c/2  b* = b      a* = -a  b* = c/2
Origin at 0,0,z        Origin at x,0,0        Origin at 0,y,0
Origin at \( \bar{1} \) on 1ca

Asymmetric unit: \( 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \)

Symmetry Operations

For \((0,0,0)\) + set

1. \( (1) \quad 1 \quad (1 | 0,0,0) \)
2. \( (2) \quad 2' \quad 1/4,0,z \quad (2_z | 1/2,0,0) \)
3. \( (3) \quad 2'' \quad 0,y,1/4 \quad (2_z | 0,0,1/2) \)
4. \( (4) \quad 2'(1/2,0,0) \quad x,0,1/4 \quad (2_z | 1/2,0,1/2) \)

5. \( (5) \quad 0,0,0 \quad (1 | 0,0,0) \)
6. \( (6) \quad a \quad (1/2,0,0) \quad x,y,0 \quad (m_z | 1/2,0,0) \)
7. \( (7) \quad c \quad (0,0,1/2) \quad x,0,z \quad (m_y | 0,0,1/2) \)
8. \( (8) \quad c' \quad (0,0,1/2) \quad 1/4,y,z \quad (m_z | 1/2,0,1/2) \)

For \((0,1,0)\)' + set

1. \( (1) \quad t' \quad (0,1,0) \quad (1 | 0,1,0) \)
2. \( (2) \quad 2' \quad 1/4,1/2,z \quad (2_z | 1/2,1/2) \)
3. \( (3) \quad 2' \quad (0,1,0) \quad 0,y,1/4 \quad (2_z | 0,1,1/2) \)
4. \( (4) \quad 2'(1/2,0,0) \quad x,1/2,1/4 \quad (2_z | 1/2,1,1/2) \)

5. \( (5) \quad 0,1/2,0 \quad (1 | 0,1,0) \)
6. \( (6) \quad n' \quad (1/2,1,0) \quad x,y,0 \quad (m_z | 1/2,1,0) \)
7. \( (7) \quad c' \quad (0,0,1/2) \quad x,1/2,z \quad (m_y | 0,1,1/2) \)
8. \( (8) \quad n' \quad (0,1,1/2) \quad 1/4,y,z \quad (m_z | 1/2,1,1/2) \)
Generators selected  (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  Coordinates  
Wyckoff letter,  Site Symmetry.

(0,0,0) +  (0,1,0)' +  

16 f 1  (1) x,y,z [u,v,w]  (2) x + 1/2,y,0 [u,v,0]  (3) x,y,z + 1/2 [u,v,w]  (4) x + 1/2,y,z + 1/2 [u,v,w]  
(5) x,y,z [u,v,w]  (6) x + 1/2,y,z [u,v,w]  (7) x,y,z + 1/2 [u,v,w]  (8) x + 1/2,y,z + 1/2 [u,v,w]  
8 e .2'  1/4,1/2,z [u,v,0]  3/4,1/2,z + 1/2 [u,v,0]  3/4,1/2,z [u,v,0]  1/4,1/2,z + 1/2 [u,v,0]  
8 d .2  1/4,0,z [0,0,w]  3/4,0,z + 1/2 [0,0,w]  3/4,0,z [0,0,w]  1/4,0,z + 1/2 [0,0,w]  
8 c .2  0,y,1/4 [0,v,0]  1/2,y,1/4 [0,v,0]  0,y,3/4 [0,v,0]  1/2,y,3/4 [0,v,0]  
8 b .1  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  
8 a .1  0,0,0 [u,v,w]  1/2,0,0 [u,v,w]  0,1/2 [u,v,w]  1/2,0,1/2 [u,v,w]  

Symmetry of Special Projections

Along [0,0,1]  p c 2mm  
Along [1,0,0]  p c 2mm  
Along [0,1,0]  p 2mg 1'  

a' = a/2  b' = b  
a' = b  b' = c/2  
a' = -a  b' = c/2  
Origin at 1/4,0,z  
Origin at x,1/2,0  
Origin at 0,y,0  

54.10.437 - 2 - 865
Ortorhombic

$P_{2b} \text{ c'}ca$

54.11.438

$mmm1'$

$P_{2b} 2_1/c'2'/c2'/a$

Origin at $\bar{1}$ on 1ca

Asymmetric unit

$0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2$

Symmetry Operations

For $(0,0,0)$ + set

(1) $1$
    $(1 | 0,0,0)$

(2) $2'$ 1/4,0,z
    $(2_x | 1/2,0,0)'$

(3) $2'$ 0,y,1/4
    $(2_x | 0,0,1/2)'$

(4) $2' (1/2,0,0) \times,0,1/4$
    $(2_x | 1/2,0,1/2)$

(5) $\bar{1}$ 0,0,0
    $(\bar{1} | 0,0,0)'$

(6) $a$ (1/2,0,0) x,y,0
    $(m_x | 1/2,0,0)$

(7) $c$ (0,0,1/2) x,0,z
    $(m_y | 0,0,1/2)$

(8) $c'$ (0,0,1/2) 1/4,y,z
    $(m_z | 1/2,0,1/2)'$

For $(0,1,0)'$ + set

(1) $t'$ (0,1,0)
    $(1 | 0,1,0)'$

(2) $2$ 1/4,1/2,z
    $(2_x | 1/2,1,0)$

(3) $2$ (0,1,0) 0,y,1/4
    $(2_x | 0,1,1/2)$

(4) $2' (1/2,0,0) \times,1/2,1/4$
    $(2_x | 1/2,1,1/2)'$

(5) $\bar{1}$ 0,1/2,0
    $(\bar{1} | 0,1,0)$

(6) $n'$ (1/2,1,0) x,y,0
    $(m_x | 1/2,1,0)'$

(7) $c' (0,0,1/2) x,1/2,z$
    $(m_y | 0,1,1/2)'$

(8) $n$ (0,1,1/2) 1/4,y,z
    $(m_z | 1/2,1,1/2)$
**Generators selected**  
(1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<tr>
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<tr>
<td>16 f 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(0,1,0)' +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) x,y,z+1/2 [u,v,w]</td>
<td>(4) x+1/2,y,z+1/2 [u,v,w]</td>
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<td>3/4,1/2,z+1/2 [0,0,w]</td>
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</tr>
<tr>
<td>8 c .2'</td>
<td>3/4,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 b 1</td>
<td>1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>8 a 1</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]** p₁c₂mm  
  \( a^* = a/2 \quad b^* = b \)  
  Origin at 0,0,z

- **Along [1,0,0]** p₂₂₁  
  \( a^* = b \quad b^* = c/2 \)  
  Origin at x,0,0

- **Along [0,1,0]** p 2mg  
  \( a^* = -a \quad b^* = c/2 \)  
  Origin at 0,y,0
**Origin** at \( \mathbf{1}^\dagger \) on 1ca'

**Asymmetric unit**

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \( (1|0,0,0) \)
2. \( \mathbf{2} \quad \frac{1}{4},0,z \)
   \( \left(2_z \mid 1/2,0,0\right) \)
3. \( \mathbf{2}' \quad 0,y,1/4 \)
   \( \left(2_y,0,1/2\right)' \)
4. \( \mathbf{2}' \quad (1/2,0,0) \quad x,0,1/4 \)
   \( \left(2_x,1/2,0,1/2\right)' \)
5. \( \mathbf{1}^\dagger \quad 0,0,0 \)
6. \( \mathbf{a}' \quad (1/2,0,0) \quad x,y,0 \)
   \( \left(m_z,1/2,0,0\right)' \)
7. \( \mathbf{c} \quad (0,0,1/2) \quad x,0,z \)
   \( \left(m_y,0,0,1/2\right) \)
8. \( \mathbf{c} \quad (0,0,1/2) \quad 1/4,y,z \)
   \( \left(m_y,1/2,0,1/2\right) \)

For \((0,1,0)'\) + set

1. \( \mathbf{t}' \quad (0,1,0) \)
   \( \left(\mathbf{1},1/2,0,0\right)' \)
2. \( \mathbf{2}' \quad 1/4,1/2,z \)
   \( \left(2_z,1/2,1,0\right)' \)
3. \( \mathbf{2} \quad (0,1,0) \quad 0,y,1/4 \)
   \( \left(2_y,0,1,1/2\right) \)
4. \( \mathbf{2} \quad (1/2,0,0) \quad x,1/2,1/4 \)
   \( \left(2_x,1/2,1,1/2\right) \)
5. \( \mathbf{1}^\dagger \quad 0,1/2,0 \)
   \( \left(\mathbf{1},1,0\right) \)
6. \( \mathbf{n} \quad (1/2,1,0) \quad x,y,0 \)
   \( \left(m_z,1/2,1,0\right) \)
7. \( \mathbf{c}' \quad (0,0,1/2) \quad x,1/2,z \)
   \( \left(m_y,0,1,1/2\right)' \)
8. \( \mathbf{n}' \quad (0,1,1/2) \quad 1/4,y,z \)
   \( \left(m_y,1/2,1,1/2\right)' \)
Generators selected  (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions  
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>16 f 1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x+1/2,y,z [u,v,w]</th>
<th>(3) x,y,z+1/2 [u,v,w]</th>
<th>(4) x+1/2,y,z+1/2 [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z [u,v,w]</td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
<td>(8) x+1/2,y,z+1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>8 e ..2'</td>
<td>1/4,1/2,z [u,v,0]</td>
<td>3/4,1/2,z+1/2 [u,v,0]</td>
<td>3/4,1/2,z [u,v,0]</td>
<td>1/4,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>8 d ..2</td>
<td>1/4,0,z [0,0,w]</td>
<td>3/4,0,z+1/2 [0,0,w]</td>
<td>3/4,0,z [0,0,w]</td>
<td>1/4,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>8 c ..2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td>1/2,y,1/4 [u,0,w]</td>
<td>0,y,3/4 [u,0,w]</td>
<td>1/2,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>8 b 1</td>
<td>0,1/2,0 [u,v,w]</td>
<td>1/2,1/2,0 [u,v,0]</td>
<td>0,1/2,1/2 [u,v,0]</td>
<td>1/2,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>8 a 1'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2a2mm  
ah^* = -b  b^* = a/2  
Origin at 0,0,z

Along [1,0,0]  p2b2mm  
a^* = b  b^* = c/2  
Origin at x,1/2,1/4

Along [0,1,0]  p 2mg1'  
a^* = -a  b^* = c/2  
Origin at 0,y,0
**P2b c’ca’**

- Origin at 1 on 1ca’
- Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

1. \( T \) (0,0,0)
2. \( T' \) (1/2,0,0)
3. \( T \) (0,0,0) (1)
4. \( T' \) (1/2,0,0) (2)
5. \( T \) (0,0,0) (3)
6. \( T' \) (1/2,0,0) (4)

For (0,1,0)’ + set

1. \( T' \) (0,1,0)
2. \( T' \) (1/2,0,0)
3. \( T' \) (0,1,0)
4. \( T' \) (0,1,0)
5. \( T' \) (1/2,0,0)
6. \( T' \) (1/2,0,0)
7. \( T' \) (0,0,0)
8. \( T' \) (0,0,0)
Generators selected  (1); t(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicty, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(0,1,0') +</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 e</td>
<td>.2</td>
<td>1/4,1/2,z [0,0,w]</td>
<td>3/4,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 d</td>
<td>.2'</td>
<td>1/4,0,z [u,v,0]</td>
<td>3/4,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 c</td>
<td>.2</td>
<td>0,y,1/4 [0,v,0]</td>
<td>1/2,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 b</td>
<td>1</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>8 a</td>
<td>1</td>
<td>0,0,0 [u,v,w]</td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1]  p_{2a}2m'm'
Along [1,0,0]  p_{2a}2'-m'm'
Along [0,1,0]  p 2mg1'

Origin at 0,0,z
Origin at x,1/2,0
Origin at 0,y,0
Origin at center (2/m)

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations:

1. 1 (1|0,0,0)
2. 2 0,0,z (2|0,0,0)
3. 2 (0,1/2,0) 1/4,y,0 (2|1/2,1/2,0)
4. 2 (1/2,0,0) x,1/4,0 (2|1/2,1/2,0)
5. T 0,0,0 (1|0,0,0)
6. m x,y,0 (m|0,0,0)
7. a (1/2,0,0) x,1/4,z (m|1/2,1/2,0)
8. b (0,1/2,0) 1/4,y,z (m|1/2,1/2,0)
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) $x',y',z$ [u,v,w]</td>
</tr>
<tr>
<td>4 h ..m</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 g ..m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>4 f ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d ..2/m</td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c ..2/m</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 b ..2/m</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a ..2/m</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg1' Along [1,0,0] p2a2mm Along [0,1,0] p2a2mm

$a^* = a$ $b^* = b$ $a^* = b/2$ $b^* = c$

Origin at 0,0,z Origin at x,1/4,0 Origin at 1/4,y,0
Origin at center (2/m1’)

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For 1 + set

1. \(1\)
   \((1|0,0,0)\)
2. \(2\)
   \((2|0,0,z)\)
3. \(2\) \((0,1/2,0)\)
   \(1/4,y,0\)
   \((2|1/2,1/2,0)\)
4. \(2\) \((1/2,0,0)\)
   \(x,1/4,0\)
   \((2|1/2,1/2,0)\)
5. \(T\) \((0,0,0)\)
6. \(m\)
   \((x,y,0)\)
   \((m,z|0,0,0)\)
7. \(a\) \((1/2,0,0)\)
   \(x,1/4,z\)
   \((m,z|1/2,1/2,0)\)
8. \(b\) \((0,1/2,0)\)
   \(1/4,y,z\)
   \((m,z|1/2,1/2,0)\)

For 1’ + set

1. \(1’\)
   \((1|0,0,0)’\)
2. \(2’\)
   \((2|0,0,z)’\)
3. \(2’\) \((0,1/2,0)’\)
   \(1/4,y,0\)
   \((2|1/2,1/2,0)’\)
4. \(2’\) \((1/2,0,0)’\)
   \(x,1/4,0\)
   \((2|1/2,1/2,0)’\)
5. \(T’\) \((0,0,0)’\)
6. \(m’\)
   \((x,y,0)’\)
   \((m,z|0,0,0)’\)
7. \(a’\) \((1/2,0,0)’\)
   \(x,1/4,z\)
   \((m,z|1/2,1/2,0)’\)
8. \(b’\) \((0,1/2,0)’\)
   \(1/4,y,z\)
   \((m,z|1/2,1/2,0)’\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) $\bar{x}$, $\bar{y}$, $z$ [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) $x$, $y$, $z$ [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 h .m1'</td>
<td>x,y,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 g .m1'</td>
<td>x,y,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 f .21'</td>
<td>0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e .21'</td>
<td>0,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 d .2/m1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 c .2/m1'</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b .2/m1'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a .2/m1'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg1'  Along [1,0,0] p 2mm1'  Along [0,1,0] p 2mm1'
$a^* = a$  $b^* = b$  $a^* = b/2$  $b^* = c$
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at center (2'/m)

Asymmetric unit 
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

1. 1
   (1 0,0,0)

2. 2'
   (2' 0,0,z)
   (2' 0,0,0)

3. 2'
   (2' 0,1/2,0)
   (2' 1/2,1/2,0)

4. 2
   (2 1/2,0,0)
   (x,1/4,0)
   (2 1/2,1/2,0)

5. 1'
   (1 0,0,0)
   (1 0,0,0)'

6. m
   (m x,y,0)
   (m' 0,0,0)
   (m' 0,0,0)

7. a
   (a 1/2,0,0)
   (x,1/4,0)
   (m 1/2,1/2,0)

8. b'
   (b' 0,1/2,0)
   (1/4,y,z)
   (m' 1/2,1/2,0)
Continued 55.3.443 Pb'am

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positions</td>
<td>Coordinates</td>
</tr>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]                     (2) x,y,z [u,v,w]                     (3) x+1/2,y+1/2,z [u,v,w]                     (4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]                     (6) x,y,z [u,v,w]                     (7) x+1/2,y+1/2,z [u,v,w]                     (8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 h .m</td>
<td>x,y,1/2 [0,0,w]                       x,y,1/2 [0,0,w]                       x+1/2,y+1/2,1/2 [0,0,w]                       x+1/2,y+1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 g .m</td>
<td>x,y,0 [0,0,w]                         x,y,0 [0,0,w]                         x+1/2,y+1/2,0 [0,0,w]                         x+1/2,y+1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 f .2'</td>
<td>0,1/2,z [u,v,0]                       1/2,0,z [u,v,0]                       0,1/2,z [u,v,0]                               1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 e .2'</td>
<td>0,0,z [u,v,0]                         1/2,1/2,z [u,v,0]                    0,0,z [u,v,0]                               1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>2 d .2'/m</td>
<td>0,1/2,1/2 [0,0,0]                     1/2,0,1/2 [0,0,0]                    1/2,0,1/2 [0,0,0]                             1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c .2'/m</td>
<td>0,1/2,0 [0,0,0]                       1/2,0,0 [0,0,0]                     1/2,0,0 [0,0,0]                               1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b .2'/m</td>
<td>0,0,1/2 [0,0,0]                       1/2,1/2,1/2 [0,0,0]                 1/2,1/2,1/2 [0,0,0]                           1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a .2'/m</td>
<td>0,0,0 [0,0,0]                         1/2,1/2,0 [0,0,0]                   1/2,1/2,0 [0,0,0]                             1/2,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>p2gg1'</td>
<td>p 2mm</td>
<td>p2a, 2mm</td>
</tr>
<tr>
<td>a* = a</td>
<td></td>
<td>a* = b/2</td>
<td>a* = -a/2</td>
</tr>
<tr>
<td>b* = b</td>
<td></td>
<td>b* = c</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,0</td>
<td></td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin at center (2/m')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2, 0,0,z \\
(3) & \quad 2', (0,1/2,0), 1/4,y,0 \\
(4) & \quad 2', (1/2,0,0), x,1/4,0 \\
(5) & \quad \bar{1}, 0,0,0 \\
(6) & \quad m', x,y,0 \\
(7) & \quad a, (1/2,0,0), x,1/4,z \\
(8) & \quad b, (0,1/2,0), 1/4,y,z \\
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x+1/2,y+1/2,z [u,v,w] (4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) x+1/2,y+1/2,z [u,v,w] (8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 h ..m'</td>
<td>x,y,1/2 [u,v,0] x,y,1/2 [u,v,0] x+1/2,y+1/2,1/2 [u,v,0] x+1/2,y+1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 g ..m'</td>
<td>x,y,0 [u,v,0] x,y,0 [u,v,0] x+1/2,y+1/2,0 [u,v,0] x+1/2,y+1/2,0 [u,v,0]</td>
</tr>
<tr>
<td>4 f ..2</td>
<td>0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 0,1/2,z [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 e ..2</td>
<td>0,0,z [0,0,w] 1/2,1/2,z [0,0,w] 0,0,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 d ..2/m'</td>
<td>0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c ..2/m'</td>
<td>0,1/2,0 [0,0,0] 1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b ..2/m'</td>
<td>0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a ..2/m'</td>
<td>0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg  Along [1,0,0] p2a 2m'm'  Along [0,1,0] p2a 2m'm'
\(a^* = a\)  \(b^* = b\)  \(a^* = b/2\)  \(b^* = c\)  \(a^* = -a/2\)  \(b^* = c\)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at center (2/m)

Asymmetric unit
\(0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}\)

Symmetry Operations

\begin{align*}
(1) \, & \, 1 \\
(1\, 0,0,0) \\
(2) \, & \, 2 \quad 0,0,z \\
(2\, z\, 0,0,0) \\
(3) \, & \, 2' \quad (0,1/2,0) \quad 1/4,y,0 \\
(2\, 1/2,1/2,0)' \\
(4) \, & \, 2' \quad (1/2,0,0) \quad x,1/4,0 \\
(2\, 1/2,1/2,0)' \\
(5) \, & \, T \\
(1\, 0,0,0) \\
(6) \, & \, m \quad x,y,0 \\
(m\, z\, 0,0,0) \\
(7) \, & \, a' \quad (1/2,0,0) \quad x,1/4,z \\
(m\, 1/2,1/2,0)' \\
(8) \, & \, b' \quad (0,1/2,0) \quad 1/4,y,z \\
(m\, 1/2,1/2,0)' 
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>4 h ..m</td>
<td>x, y, 1/2 [0, 0, w]</td>
</tr>
<tr>
<td>4 g ..m</td>
<td>x, y, 0 [0, 0, w]</td>
</tr>
<tr>
<td>4 f ..2</td>
<td>0, 1/2, z [0, 0, w]</td>
</tr>
<tr>
<td>4 e ..2</td>
<td>0, 0, z [0, 0, w]</td>
</tr>
<tr>
<td>2 d ..2/m</td>
<td>0, 1/2, 1/2 [0, 0, w]</td>
</tr>
<tr>
<td>2 c ..2/m</td>
<td>0, 1/2, 0 [0, 0, w]</td>
</tr>
<tr>
<td>2 b ..2/m</td>
<td>0, 0, 1/2 [0, 0, w]</td>
</tr>
<tr>
<td>2 a ..2/m</td>
<td>0, 0, 0 [0, 0, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2gg1'</th>
<th>Along [1,0,0]</th>
<th>p 2'mm'</th>
<th>Along [0,1,0]</th>
<th>p 2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>b* = a/2</td>
<td>a* = -c</td>
<td>b* = b/2</td>
<td>a* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (2'/m')

Asymmetric unit \[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations:

1. \( \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \)
2. \( \begin{pmatrix} 2' \\ 0 \\ 0 \\ z \end{pmatrix} \)
3. \( \begin{pmatrix} 2 \\ (0,1/2,0) \\ 1/4, y, 0 \end{pmatrix} \)
4. \( \begin{pmatrix} 2' \\ (1/2,0,0) \\ x, 1/4, 0 \end{pmatrix} \)
5. \( \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \)
6. \( \begin{pmatrix} m' \\ x, y, 0 \end{pmatrix} \)
7. \( \begin{pmatrix} a \\ (1/2,0,0) \\ x, 1/4, z \end{pmatrix} \)
8. \( \begin{pmatrix} b' \\ (0,1/2,0) \\ 1/4, y, z \end{pmatrix} \)

\( \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 h ..m' x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 g ..m' x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,0 [u,v,0]</td>
</tr>
<tr>
<td>4 f ..2' 0,1/2,z [u,v,0]</td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [u,v,0]</td>
</tr>
<tr>
<td>4 e ..2' 0,0,z [u,v,0]</td>
<td>1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>2 d ..2'/m' 0,1/2,1/2 [u,v,0]</td>
<td>1/2,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2 c ..2'/m' 0,1/2,0 [u,v,0]</td>
<td>1/2,0,0 [u,v,0]</td>
</tr>
<tr>
<td>2 b ..2'/m' 0,0,1/2 [u,v,0]</td>
<td>1/2,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2 a ..2'/m' 0,0,0 [u,v,0]</td>
<td>1/2,1/2,0 [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2'gg'</th>
<th>Along [1,0,0] p 2'mm'</th>
<th>Along [0,1,0] p2x 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b  b* = a</td>
<td>a* = b/2  b* = c</td>
<td>a* = -a/2  b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 1/4,y,0</td>
</tr>
</tbody>
</table>
Origin at center (2/m')

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

1. \( \begin{align*} 1 \\ (1 | 0,0,0) \end{align*} \)
2. \( \begin{align*} 2 & 0,0,z \\ (2_z | 0,0,0) \end{align*} \)
3. \( \begin{align*} 2 & (0,1/2,0) 1/4,y,0 \\ (2_{y} | 1/2,1/2,0) \end{align*} \)
4. \( \begin{align*} 2 & (1/2,0,0) x,1/4,0 \\ (2_{x} | 1/2,1/2,0) \end{align*} \)
5. \( \begin{align*} \bar{1} & 0,0,0 \\ (\bar{1} | 0,0,0)' \end{align*} \)
6. \( \begin{align*} m' & x,y,0 \\ (m_{z} | 0,0,0)' \end{align*} \)
7. \( \begin{align*} a' & (1/2,0,0) x,1/4,z \\ (m_{y} | 1/2,1/2,0)' \end{align*} \)
8. \( \begin{align*} b' & (0,1/2,0) 1/4,y,z \\ (m_{x} | 1/2,1/2,0)' \end{align*} \)
Continued

55.7.447

Pb'a'm'

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 h .m'</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 g .m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,0 [u,v,0]</td>
</tr>
<tr>
<td>4 f .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1 [0,0,w]</td>
</tr>
<tr>
<td>4 e .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 d .2/m'</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c .2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b .2/m'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a .2/m'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2g'g'</th>
<th>Along [1,0,0]</th>
<th>p 2m'm'</th>
<th>Along [0,1,0]</th>
<th>p 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a</td>
<td></td>
<td>b' = b</td>
<td></td>
<td>a' = c</td>
<td></td>
</tr>
<tr>
<td>b' = b</td>
<td></td>
<td>c' = c</td>
<td></td>
<td>a' = c</td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center (2/m)

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1) 1
   (1|0,0,0)

2) 2 0,0,z
   (Z|0,0,0)

3) 2 (0,1/2,0) 1/4,y,0
   (Z|1/2,1/2,0)

4) 2 (1/2,0,0) x,1/4,0
   (Z|1/2,1/2,0)

5) 1
   (0,0,0)

6) m x,y,0
   (m|0,0,0)

7) a (1/2,0,0) x,1/4,z
   (m|1/2,1/2,0)

8) b (0,1/2,0) 1/4,y,z
   (m|1/2,1/2,0)

For (0,0,1)’ + set

1) t’ (0,0,1)
   (1|0,0,1)’

2) 2’ (0,0,1) 0,0,z
   (Z|0,0,1)’

3) 2’ (0,1/2,0) 1/4,y,1/2
   (Z|1/2,1/2,1)’

4) 2’ (1/2,0,0) x,1/4,1/2
   (Z|1/2,1/2,1)’

5) 1’ 0,0,1/2
   (1|0,0,1)’

6) m’ x,y,1/2
   (m|0,0,1)’

7) n’ (1/2,0,1) x,1/4,z
   (m|1/2,1/2,1)’

8) n’ (0,1/2,1) 1/4,y,z
   (m|1/2,1/2,1)’
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (0,0,1)’ +</td>
</tr>
<tr>
<td>16 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 h m’n</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 g m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 f 2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 e 2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 d 2/m’</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c 2/m</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 b 2/m’</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2/m</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2gg1’
  - $a^* = a$  
  - $b^* = b$
- Along [1,0,0] p_ce 2mm
  - $a^* = b/2$  
  - $b^* = c$
- Along [0,1,0] p_ce 2mm
  - $a^* = c$  
  - $b^* = a/2$

**Origin**
- Origin at 0,0,z
- Origin at x,1/4,0
- Origin at 1/4,y,0
Orthorhombic

Origin at center \((2/m)\)

Asymmetric unit

\[ 0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/2 \]

Symmetry Operations

For \((0,0,0) + set\)

1. \(1\) \((0,0,0)\)

2. \(2'\) \((0,0,z)\)
\((2_z,0,0,0)'\)

3. \(2'\) \((0,1/2,0)\) \((1/4,y,0)\)
\((2_y,1/2,1/2,0)'\)

4. \(2\) \((1/2,0,0)\) \((x,1/4,0)\)
\((2_x,1/2,1/2,0)'\)

5. \(1'\) \((0,0,0)\)

6. \(m\) \((x,y,0)\)
\((m_y,1/2,1/2,0)'\)

7. \(a\) \((1/2,0,0)\) \((x,1/4,z)\)
\((m_x,1/2,1/2,0)'\)

8. \(b'\) \((0,1/2,0)\) \((1/4,y,z)\)
\((m_x,1/2,1/2,0)'\)

For \((0,0,1) + set\)

1. \(t'\) \((0,0,1)\)
\((1,0,0,1)'\)

2. \(2\) \((0,0,1)\) \((0,0,z)\)
\((2_z,0,0,1)'\)

3. \(2\) \((0,1/2,0)\) \((1/4,y,1/2)\)
\((2_y,1/2,1/2,1)'\)

4. \(2'\) \((1/2,0,0)\) \((x,1/4,1/2)\)
\((2_x,1/2,1/2,1)'\)

5. \(1\) \((0,0,1/2)\)
\((1,0,0,1)'\)

6. \(m'\) \((x,y,1/2)\)
\((m_y,1/2,1/2,1)'\)

7. \(n'\) \((1/2,0,1)\) \((1/4,z)\)
\((m_y,1/2,1/2,1)'\)

8. \(n\) \((0,1/2,1)\) \((1/4,y,z)\)
\((m_x,1/2,1/2,1)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

(0,0,0) + (0,0,1)'

16 i 1 (1) x,y,z [u,v,w] (2) x',y',z [u,v,w] (3) x+1/2,y+1/2,z' [u,v,w] (4) x+1/2,y+1/2,z [u,v,w]

8 h .m' x,y,1/2 [u,v,0] x',y,1/2 [u,v,0] x+1/2,y+1/2,1/2 [u,v,0] x+1/2,y+1/2,1/2 [u,v,0]

8 g .m x,y,0 [0,0,w] x',y,0 [0,0,w] x+1/2,y+1/2,0 [0,0,w] x+1/2,y+1/2,0 [0,0,w]

8 f ..2' 0,1/2,z [u,v,0] 1/2,0,z [u,v,0] 0,1/2,z [u,v,0] 1/2,0,z [u,v,0]

8 e ..2' 0,0,z [u,v,0] 1/2,1/2,z [u,v,0] 0,0,z [u,v,0] 1/2,1/2,z [u,v,0]

4 d ..2/m' 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]

4 c ..2/m 0,1/2,0 [0,0,0] 1/2,0,0 [0,0,0]

4 b ..2/m' 0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]

4 a ..2/m' 0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2gg1'  Along [1,0,0] p_{2c} 2mm  Along [0,1,0] p_{2c} 2mm

a* = a  b* = b  a* = -c  b* = b/2  a* = c  b* = a/2

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Orthorhombic

\[ 55.10.450 \]

\[ P_{\text{2c} b' a'm} \]

\[ mmm1' \]

\[ P_{2c 2' b' 2', a'2'm} \]

**Origin** at center (\( 2/m \))

**Asymmetric unit**

\[ 0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/2 \]

**Symmetry Operations**

**For \((0,0,0) + \) set**

1. \((1|0,0,0)\)
2. \((2|0,0,z)\)
3. \((3|0,1/2,0)\)
4. \((4|1/2,0,0)\)
5. \((5|0,0,0)\)
6. \((6|1/2,1/2,0)^*\)
7. \((7|1/2,1/2,1)^*\)
8. \((8|1/2,1/2,0)^*\)

**For \((0,0,1') + \) set**

1. \((1|0,0,1')\)
2. \((2|0,0,1)\)
3. \((3|0,1/2,0)\)
4. \((4|1/2,0,0)\)
5. \((5|0,0,1/2)\)
6. \((6|0,0,1)\)
7. \((7|1/2,0,1)\)
8. \((8|0,1/2,1)\)

\[ 55.10.450 - 1 - 890 \]
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>(0,0,0)</td>
<td>(0,0,0) + (0,0,1)' +</td>
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<tr>
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<td>i 1</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>(3) x+1/2, y+1/2, z [u, v, w]</td>
<td>(4) x+1/2, y+1/2, z [u, v, w]</td>
</tr>
<tr>
<td>(5) x, y, z [u, v, w]</td>
<td>(6) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>(7) x+1/2, y+1/2, z [u, v, w]</td>
<td>(8) x+1/2, y+1/2, z [u, v, w]</td>
</tr>
<tr>
<td>8</td>
<td>h ..m'</td>
</tr>
<tr>
<td>x, y, 1/2 [u, v, 0]</td>
<td>x, y, 1/2 [u, v, 0]</td>
</tr>
<tr>
<td>x+1/2, y+1/2, 1/2 [u, v, 0]</td>
<td>x+1/2, y+1/2, 1/2 [u, v, 0]</td>
</tr>
<tr>
<td>8</td>
<td>g ..m</td>
</tr>
<tr>
<td>x, y, 0 [0, 0, w]</td>
<td>x, y, 0 [0, 0, w]</td>
</tr>
<tr>
<td>x+1/2, y+1/2, 0 [0, 0, w]</td>
<td>x+1/2, y+1/2, 0 [0, 0, w]</td>
</tr>
<tr>
<td>8</td>
<td>f ..2</td>
</tr>
<tr>
<td>0, 1/2, z [0, 0, w]</td>
<td>1/2, 0, z [0, 0, w]</td>
</tr>
<tr>
<td>0, 1/2, z [0, 0, w]</td>
<td>1/2, 0, z [0, 0, w]</td>
</tr>
<tr>
<td>8</td>
<td>e ..2</td>
</tr>
<tr>
<td>0, 0, z [0, 0, w]</td>
<td>1/2, 1/2, z [0, 0, w]</td>
</tr>
<tr>
<td>0, 0, z [0, 0, w]</td>
<td>1/2, 1/2, z [0, 0, w]</td>
</tr>
<tr>
<td>4</td>
<td>d ..2/m'</td>
</tr>
<tr>
<td>0, 1/2, 1/2 [0, 0, 0]</td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>4</td>
<td>c ..2/m</td>
</tr>
<tr>
<td>0, 1/2, 0 [0, 0, w]</td>
<td>1/2, 0, 0 [0, 0, w]</td>
</tr>
<tr>
<td>4</td>
<td>b ..2/m'</td>
</tr>
<tr>
<td>0, 0, 1/2 [0, 0, 0]</td>
<td>1/2, 1/2, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>4</td>
<td>a ..2/m</td>
</tr>
<tr>
<td>0, 0, 0 [0, 0, w]</td>
<td>1/2, 1/2, 0 [0, 0, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2gg1'  Along [1,0,0]  p2a2' 2m'm'  Along [0,1,0]  p2a2' 2m'm'

| a* = a | b* = b |
| a* = -c | b* = b/2 |
| Origin at 0,0,z | Origin at x,0,1/2 |

| a* = c | b* = a/2 |
| a* = -c | b* = b/2 |
| Origin at 1/4,y,1/2 | Origin at x,0,1/2 |
Origin at $\overline{1}$ on 11n

Asymmetric unit: $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$

Symmetry Operations:

1. $1 (1 | 0,0,0)$
2. $2 1/4,1/4,z (2 \overline{z} | 1/2,1/2,0)$
3. $2 (0,1/2,0) 0,y,1/4 (2 | 0,1/2,1/2)$
4. $2 (1/2,0,0) x,0,1/4 (2 | 1/2,0,1/2)$
5. $\overline{1} 0,0,0 (1 | 0,0,0)$
6. $n (1/2,1/2,0) x,y,0 (m_{\overline{z}} | 1/2,1/2,0)$
7. $c (0,0,1/2) x,1/4,z (m_{y} | 0,1/2,1/2)$
8. $c (0,0,1/2) 1/4,y,z (m_{z} | 1/2,0,1/2)$
Continued

Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
8 & \quad e & 1 & \quad (1) & x,y,z & [u,v,w] & \quad (2) & x+1/2, y+1/2, z & [u,v,w] & \quad (3) & x, y+1/2, z+1/2 & [u,v,w] & \quad (4) & x+1/2, y, z+1/2 & [u,v,w] \\
& & & & \quad (5) & x, y, z & [u,v,w] & \quad (6) & x+1/2, y+1/2, z & [u,v,w] & \quad (7) & x, y+1/2, z+1/2 & [u,v,w] & \quad (8) & x+1/2, y, z+1/2 & [u,v,w] \\
4 & \quad d & 0.2 & \quad 1/4, 3/4, z & [0,0,w] & \quad 3/4, 1/4, z+1/2 & [0,0,w] & \quad 3/4, 1/4, z & [0,0,w] & \quad 1/4, 3/4, z+1/2 & [0,0,w] \\
4 & \quad c & 0.2 & \quad 1/4, 1/4, z & [0,0,w] & \quad 3/4, 3/4, z+1/2 & [0,0,w] & \quad 3/4, 3/4, z & [0,0,w] & \quad 1/4, 1/4, z+1/2 & [0,0,w] \\
4 & \quad b & 1 & \quad 0, 0, 1/2 & [u,v,w] & \quad 1/2, 1/2, 1/2 & [u,v,w] & \quad 0, 1/2, 0 & [u,v,w] & \quad 1/2, 0, 0 & [u,v,w] \\
4 & \quad a & 1 & \quad 0, 0, 0 & [u,v,w] & \quad 1/2, 1/2, 0 & [u,v,w] & \quad 0, 1/2, 1/2 & [u,v,w] & \quad 1/2, 0, 1/2 & [u,v,w] \\
\end{align*}
\]

Symmetry of Special Projections

Along \([0,0,1]\) \( c_{1p}, 2mm \)  
Along \([1,0,0]\) \( p_{21b}, 2m'g' \)  
Along \([0,1,0]\) \( p_{21b}, 2m'g' \)

\[
\begin{align*}
a^* & = a & b^* & = b & \quad a^* & = b & b^* & = c/2 & \quad a^* & = -a & b^* & = c/2 \\
\end{align*}
\]

Origin at \(1/4, 1/4, z\)  
Origin at \(x, 0, 1/4\)  
Origin at \(0, y, 0\)
Origin at \(1'\) on 11\(n1'\)

Asymmetric unit \(0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{2}\)

Symmetry Operations

For 1 + set

1. \((0,0,0)\)
2. \((1/4,1/4,z)\)
3. \((0,1/2,0)\)
4. \((1/2,0,0)\)
5. \((0,0,0)\)
6. \((1/2,1/2,0)\)
7. \((0,0,1/2)\)
8. \((0,0,1/2)\)

For \(1'\) + set

1. \((0,0,0)\)
2. \((1/4,1/4,z)\)
3. \((0,1/2,0)\)
4. \((1/2,0,0)\)
5. \((0,0,0)\)
6. \((1/2,1/2,0)\)
7. \((0,0,1/2)\)
8. \((0,0,1/2)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

Multiplicity,  Coordinates
Wyckoff letter,  Site Symmetry.

<p>|</p>
<table>
<thead>
<tr>
<th>1</th>
<th>1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>36</td>
<td>---</td>
</tr>
</tbody>
</table>

| 8 e  | 11' | (1) x,y,z [0,0,0]  (2) x+1/2,y+1/2,z [0,0,0]  (3) x,y+1/2,z+1/2 [0,0,0]  (4) x+1/2,y,z+1/2 [0,0,0]  (5) x,y,z [0,0,0]  (6) x+1/2,y+1/2,z [0,0,0]  (7) x,y+1/2,z+1/2 [0,0,0]  (8) x+1/2,y,z+1/2 [0,0,0]  |
| 4 d  | .21' | 1/4,3/4,z [0,0,0]  3/4,1/4,z+1/2 [0,0,0]  3/4,1/4,z [0,0,0]  1/4,3/4,z+1/2 [0,0,0]  |
| 4 c  | .21' | 1/4,1/4,z [0,0,0]  3/4,3/4,z+1/2 [0,0,0]  3/4,3/4,z [0,0,0]  1/4,1/4,z+1/2 [0,0,0]  |
| 4 b  | 11' | 0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]  |
| 4 a  | 11' | 0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  |

Symmetry of Special Projections

Along [0,0,1]  c2mm1'  Along [1,0,0]  p 2mg1'  Along [0,1,0]  p 2mg1'
a* = a  b* = b  a* = b  b* = c/2  a* = -a  b* = c/2
Origin at 1/4,1/4,z  Origin at x,0,0  Origin at 0,y,0
Pc'cn

56.3.453

m'mm

P2₁, /c'2, '/c2'/n

Orthorhombic

Origin at \( \bar{1} \) on \( 11n \)

Asymmetric unit

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. \[ 1 \]
2. \[ 2', 1/4, 1/4, z \]
3. \[ 2', (0, 1/2, 0), 0, y, 1/4 \]
4. \[ 2, (1/2, 0, 0), x, 0, 1/4 \]
5. \[ \bar{1}, 0, 0, 0 \]
6. \[ n, (1/2, 1/2, 0), x, y, 0 \]
7. \[ c, (0, 0, 1/2), x, 1/4, z \]
8. \[ c', (0, 0, 1/2), 1/4, y, z \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w] (2) x+1/2,y+1/2,z [u,v,w] (3) x,y+1/2,z+1/2 [u,v,w] (4) x+1/2,y,z+1/2 [u,v,w] (5) x,y,z [u,v,w] (6) x+1/2,y+1/2,z [u,v,w] (7) x,y+1/2,z+1/2 [u,v,w] (8) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 d .2'</td>
<td>1/4,3/4,z [u,v,0] 3/4,1/4,z+1/2 [u,v,0] 3/4,1/4,z [u,v,0] 1/4,3/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>1/4,1/4,z [u,v,0] 3/4,3/4,z+1/2 [u,v,0] 3/4,3/4,z [u,v,0] 1/4,1/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b 1'</td>
<td>0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 0,1/2,0 [0,0,0] 1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1'</td>
<td>0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c_p 2'mm'

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>c_p 2'mm'</td>
</tr>
<tr>
<td>a' = a  b' = b</td>
<td>Origin at 1/4,1/4,z</td>
</tr>
</tbody>
</table>

Along [1,0,0]  p 2mg

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,0,0]</td>
<td>p 2mg</td>
</tr>
<tr>
<td>a' = b  b' = c/2</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>

Along [0,1,0]  p_2b 2mg

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,1,0]</td>
<td>p_2b 2mg</td>
</tr>
<tr>
<td>a' = -a  b' = c/2</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>

56.3.453 - 2 - 897
Origin at \( \bar{1} \) on \( 11 \) column

Asymmetric unit

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. \( 1 \)
   - \( (1|0,0,0) \)
   - \( (1|0,0,0)' \)

2. \( 2 \)
   - \( 1/4,1/4,z \)
   - \( 1/2,1/2,0 \)

3. \( 2' \)
   - \( 0,1/2,0 \)
   - \( x,y,1/4 \)
   - \( 0,1/2,1/2 \)

4. \( 2' \)
   - \( 1/2,0,0 \)
   - \( x,0,1/4 \)
   - \( 1/2,0,1/2 \)

5. \( \bar{1} \)
   - \( 0,0,0 \)

6. \( n' \)
   - \( 1/2,1/2,0 \)
   - \( x,y,0 \)
   - \( 1/2,1/2,0 \)

7. \( c \)
   - \( 0,0,1/2 \)
   - \( x,1/4,z \)
   - \( 0,1/2,1/2 \)

8. \( m \)
   - \( 0,0,1/2 \)
   - \( 1/4,y,z \)
   - \( 0,1/2,0 \)

- \( 1 \) is the identity operation.
- \( 2 \) represents a 90° rotation about the x-axis.
- \( 2' \) represents a 90° rotation about the y-axis.
- \( \bar{1} \) represents a reflection in the plane perpendicular to the x-axis.
- \( n' \) represents a 180° rotation about the z-axis.
- \( c \) represents a glide reflection along the z-axis.
- \( m \) represents a screw operation.
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

4 d ..2  
1/4,3/4,z [0,0,w]  
3/4,1/4,z+1/2 [0,0,w]  
3/4,1/4,z [0,0,w]  
1/4,3/4,z+1/2 [0,0,w]  

4 c ..2  
1/4,1/4,z [0,0,w]  
3/4,3/4,z+1/2 [0,0,w]  
3/4,3/4,z [0,0,w]  
1/4,1/4,z+1/2 [0,0,w]  

4 b 1'  
0,0,1/2 [0,0,0]  
1/2,1/2,1/2 [0,0,0]  
0,1/2,0 [0,0,0]  
1/2,0,0 [0,0,0]  

4 a 1'  
0,0,0 [0,0,0]  
1/2,1/2,0 [0,0,0]  
0,1/2,1/2 [0,0,0]  
1/2,0,1/2 [0,0,0]  

**Symmetry of Special Projections**

Along [0,01] c2mm  
Along [1,0,0] p21b, 2m'g'  
Along [0,1,0] p21b, 2m'g'  

\[ a^* = a \quad b^* = b \]  
\[ a^* = b \quad b^* = c/2 \]  
\[ a^* = -a \quad b^* = c/2 \]  

Origin at 1/4,1/4,z  
Origin at x,0,0  
Origin at 0,y,0
**Origin** at $\vec{1}$ on 11n

**Asymmetric unit**  
$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

1. $I$  
   (1) $I$  
   (5) $\bar{1}$  
   (0,0,0)

2. $2$  
   (2) $2 1/4,1/4,z$  
   (2) $1/2,1/2,0$

3. $2'$  
   (3) $2' (0,1/2,0) 0,y,1/4$  
   (2,$y,0,1/2$)

4. $2'$  
   (4) $2' (1/2,0,0) x,0,1/4$  
   (2,$x,1/2,0$)

5. $\bar{1}$  
   (5) $\bar{1}$  
   (6) $n (1/2,1/2,0) x,y,0$  
   (m,$y,1/2,1/2$)

6. $\bar{1}$  
   (7) $c' (0,0,1/2) x,1/4,z$  
   (m,$y,0,1/2,1/2$)

7. $\bar{1}$  
   (8) $c' (0,0,1/2) 1/4,y,z$  
   (m,$y,1/2,0,1/2$)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 8 e 1        | (1) x,y,z [u,v,w]  
|              | (2) x+1/2,y+1/2,z [u,v,w]  
|              | (3) x,y+1/2,z+1/2 [u,v,w]  
|              | (4) x+1/2,y,z+1/2 [u,v,w]  
|              | (5) x,y,z [u,v,w]  
|              | (6) x+1/2,y+1/2,z [u,v,w]  
|              | (7) x,y+1/2,z+1/2 [u,v,w]  
|              | (8) x+1/2,y,z+1/2 [u,v,w]  |
| 4 d ..2      | 1/4,3/4,z [0,0,w]  
|              | 3/4,1/4,z+1/2 [0,0,w]  
|              | 3/4,1/4,z [0,0,w]  
|              | 1/4,3/4,z+1/2 [0,0,w]  |
| 4 c ..2      | 1/4,1/4,z [0,0,w]  
|              | 3/4,3/4,z+1/2 [0,0,w]  
|              | 3/4,3/4,z [0,0,w]  
|              | 1/4,1/4,z+1/2 [0,0,w]  |
| 4 b .1       | 0,0,1/2 [u,v,w]  
|              | 1/2,1/2,1/2 [u,v,w]  
|              | 0,1/2,0 [u,v,w]  
|              | 1/2,0,0 [u,v,w]  |
| 4 a .1       | 0,0,0 [u,v,w]  
|              | 1/2,1/2,0 [u,v,w]  
|              | 0,1/2,1/2 [u,v,w]  
|              | 1/2,0,1/2 [u,v,w]  |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>沿 [0,01] c2m'm'</th>
<th>沿 [1,0,0] p 2'm'g</th>
<th>沿 [0,1,0] p 2'm'g</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>a* = -a</td>
</tr>
<tr>
<td>b* = b</td>
<td></td>
<td>b* = c/2</td>
<td>b* = c/2</td>
</tr>
</tbody>
</table>

Origin at 1/4,1/4,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at $\bar{1}$ on 11n'

Asymmetric unit

0 \leq x \leq 1/4; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2

Symmetry Operations

1. $1$
   1
   0,0,0

2. $2'$ 1/4,1/4,z
   (2$'_z$ 1/2,1/2,0)'

3. $2$ (0,1/2,0) 0,y,1/4
   (2$_y$ 0,1/2,1/2)

4. $2'$ (1/2,0,0) x,0,1/4
   (2$'_x$ 1/2,0,1/2)'

5. $\bar{1}$ 0,0,0
   (1|0,0,0)

6. n' (1/2,1/2,0) x,y,0
   (m$'_z$ 1/2,1/2,0)'

7. c (0,0,1/2) x,1/4,z
   (m$'_y$ 0,1/2,1/2)

8. c' (0,0,1/2) 1/4,y,z
   (m$'_x$ 1/2,0,1/2)'

56.6.456 - 1 - 902
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5). \)

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>( (1) ) ( x,y,z ) [( u,v,w )]</td>
<td>( (1) ) ( x,y,z ) [( u,v,w )]</td>
</tr>
<tr>
<td>4 d ( .2' )</td>
<td>( 1/4,3/4,z ) [( u,v,0 )]</td>
<td>( 1/4,3/4,z+1/2 ) [( u,v,0 )]</td>
</tr>
<tr>
<td>4 c ( .2' )</td>
<td>( 1/4,1/4,z ) [( u,v,0 )]</td>
<td>( 1/4,1/4,z+1/2 ) [( u,v,0 )]</td>
</tr>
<tr>
<td>4 b ( \overline{1} )</td>
<td>( 0,0,1/2 ) [( u,v,w )]</td>
<td>( 0,1/2,0 ) [( u,v,w )]</td>
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<tr>
<td>4 a ( \overline{1} )</td>
<td>( 0,0,0 ) [( u,v,w )]</td>
<td>( 0,1/2,1/2 ) [( u,v,w )]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along \([0,01]\) c2\( mm'\)**
  - \( a^* = -b \quad b^* = a \)
  - Origin at \( 1/4,1/4,z \)

- **Along \([1,0,0]\) p\( 2'mg'\)**
  - \( a^* = b \quad b^* = c/2 \)
  - Origin at \( x,0,0 \)

- **Along \([0,1,0]\) \( p_{2\beta},2mg \)**
  - \( a^* = -a \quad b^* = c/2 \)
  - Origin at \( 0,y,0 \)
Origin at $\overline{1}$ on $11n'$

Asymmetric unit $0 < x < 1/4; 0 < y < 1; 0 < z < 1/2$

Symmetry Operations

1. $\begin{align*}
T & (1,0,0,0) \\
& (1,0,0,0)' \\
\end{align*}$

2. $\begin{align*}
& (2,1/4,1/4,0) \\
& (2,1/2,1/2,0) \\
\end{align*}$

3. $\begin{align*}
& (3,0,1/2,0) \\
& (3,1/2,1/2,0) \\
\end{align*}$

4. $\begin{align*}
& (4,0,1/2,0) \\
& (4,1/2,0,1/2) \\
\end{align*}$

5. $\begin{align*}
& (5,0,0,0) \\
& (5,0,0,0)' \\
\end{align*}$

6. $\begin{align*}
& (6,n',1/2,1/2) \\
& (6,m_z,1/2,1/2) \\
\end{align*}$

7. $\begin{align*}
& (7,c',0,0,1/2) \\
& (7,m_y,0,1/2,1/2) \\
\end{align*}$

8. $\begin{align*}
& (8,c',0,0,1/2) \\
& (8,m_z,1/2,0,1/2) \\
\end{align*}$

Orthorhombic
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) x,y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2, y, z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2, y+1/2, z [u,v,w]</td>
</tr>
<tr>
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<td>(7) x,y+1/2, z+1/2 [u,v,w]</td>
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<td>(8) x+1/2, y, z+1/2 [u,v,w]</td>
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<tr>
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<td>1/4,3/4,z [0,0,w]</td>
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<td>3/4,1/4,z+1/2 [0,0,w]</td>
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<td>1/4,3/4,z+1/2 [0,0,w]</td>
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<td>4 c ..2</td>
<td>1/4,1/4,z [0,0,w]</td>
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<td>1/4,1/4,z+1/2 [0,0,w]</td>
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<tr>
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<td>0,0,1/2 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>4 a 1/4</td>
<td>0,0,0 [0,0,0]</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1]  c2m'm'  
Along [1,0,0] p 2m'g'  
Along [0,1,0] p 2m'g'

\( a^* = a \quad b^* = b \)

Along [0,0,1]  c2m'm'  
Along [1,0,0] p 2m'g'  
Along [0,1,0] p 2m'g'

\( a^* = -a \quad b^* = c/2 \)
**Orthonormic**

57.1.458

Pbcm

mmm

P2/b21/c21/m

---

### Origin

At \( \vec{1} \) on \( b12 \)

### Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \]

### Symmetry Operations

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Asymmetric Domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \vec{1} )</td>
<td>( 0,0,0 )</td>
</tr>
<tr>
<td>2</td>
<td>( (0,0,1/2) )</td>
<td>( 0,0,z )</td>
</tr>
<tr>
<td>3</td>
<td>( (0,1/2,0) )</td>
<td>( 0,y,1/4 )</td>
</tr>
<tr>
<td>4</td>
<td>( (0,1/2,1/2) )</td>
<td>( 0,y,z )</td>
</tr>
<tr>
<td>5</td>
<td>( \vec{1} )</td>
<td>( 0,0,0 )</td>
</tr>
<tr>
<td>6</td>
<td>( m )</td>
<td>( x,y,1/4 )</td>
</tr>
<tr>
<td>7</td>
<td>( c )</td>
<td>( x,1/4,z )</td>
</tr>
<tr>
<td>8</td>
<td>( b )</td>
<td>( 0,1/2,0 )</td>
</tr>
</tbody>
</table>

---

[Diagram showing lattice and symmetry operations]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w] (2) (\bar{x},y,z+1/2 [u,v,w]) (3) (x,y+1/2,z+1/2 [u,v,w]) (4) (x,y+1/2,z [u,v,w]) (5) (x,y,z [u,v,w]) (6) (x,y,z+1/2 [u,v,w]) (7) (x,y+1/2,z+1/2 [u,v,w]) (8) (x,y+1/2,z [u,v,w])</td>
</tr>
<tr>
<td>4 d ..m</td>
<td>x,y,1/4 [0,0,w] (\bar{x},y,3/4 [0,0,w]) (\bar{x},y+1/2,1/4 [0,0,w]) (x,\bar{y}+1/2,3/4 [0,0,w])</td>
</tr>
<tr>
<td>4 c 2..</td>
<td>x,1/4,0 [u,0,0] (\bar{x},3/4,1/2 [u,0,0]) (\bar{x},3/4,0 [u,0,0]) (x,1/4,1/2 [u,0,0])</td>
</tr>
<tr>
<td>4 b 1</td>
<td>1/2,0,0 [u,v,w] (\bar{1},2,0,1/2 [u,v,w]) (1/2,1,2,1/2 [u,v,w]) (1/2,1,1/2,0 [u,v,w])</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w] (0,0,1/2 [u,v,w]) (0,1/2,1/2 [u,v,w]) (0,1/2,0 [u,v,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,01] \(p2mg1'\) Along [1,0,0] \(p_{2b},2mg\) Along [0,1,0] \(p_{2a},2mm\)
\(a^* = -b \quad b^* = a\) \(a^* = -c \quad b^* = b/2\) \(a^* = c/2 \quad b^* = a\)
Origin at 0,0,z Origin at x,1/4,0 Origin at 0,y,1/4
Pbcm1'  mmm1'  Orthorhombic

57.2.459  P2/b2/c2/m1'

Origin at 1' on b1211'
Asymmetric unit  0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1;  0 ≤ z ≤ 1/4

Symmetry Operations

For 1' + set

(1) 1
     (1) 1
(1) 1'
(1) 1'

(2) 2 (0,0,1/2)  0,0,z
     (2) 2 (0,0,1/2)
(2) 2'
(2) 2'

(3) 2 (0,1/2,0)  0,y,1/4
     (3) 2 (0,1/2,0)
(3) 2'
(3) 2'

(4) 2 x,1/4,0
     (4) 2 (2x,0,0,1/2,1/2)
(4) 2
(4) 2

(5) m x,y,1/4
     (5) m x,y,1/4
(5) m'
(5) m'

(6) m (0,0,0)
     (6) m (0,0,0)
(6) m
(6) m

(7) c (0,0,1/2)  x,1/4,z
     (7) c (0,0,1/2)
(7) c'
(7) c'

(8) b (0,1/2,0)  0,y,z
     (8) b (0,1/2,0)
(8) b'
(8) b'

(1') 1
     (1') 1
(1') 1'
(1') 1'

(2') 2 (0,0,1/2)  0,0,z
     (2') 2 (0,0,1/2)
(2') 2'
(2') 2'

(3') 2' (0,1/2,0)  0,y,1/4
     (3') 2' (0,1/2,0)
(3') 2''
(3') 2''

(4') 2' x,1/4,0
     (4') 2' (2x,0,0,1/2,1/2)
(4') 2'
(4') 2'

(5') m' x,y,1/4
     (5') m' x,y,1/4
(5') m''
(5') m''

(6') m' (0,0,0)
     (6') m' (0,0,0)
(6') m''
(6') m''

(7') c' (0,0,1/2)  x,1/4,z
     (7') c' (0,0,1/2)
(7') c''
(7') c''

(8') b' (0,1/2,0)  0,y,z
     (8') b' (0,1/2,0)
(8') b''
(8') b''

57.2.459 - 1 - 908
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x, y, z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [0,0,0]</td>
<td>(6) x, y, z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 d ..m1'</td>
<td>x,y,1/4 [0,0,0]</td>
<td>x,y,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c 2..1'</td>
<td>x,1/4,0 [0,0,0]</td>
<td>x,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b 11'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 11'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,01] p2mg1'  
  $a^* = -b$  $b^* = a$
  Origin at 0,0,z
- Along [1,0,0] p2mg1'  
  $a^* = -c$  $b^* = b/2$
  Origin at x,0,0
- Along [0,1,0] p2mm1'  
  $a^* = c/2$  $b^* = a$
  Origin at 0,y,0
Origin at \( \bar{1} \) on \( b'12_1' \)

Asymmetric unit  \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \quad (1 \mid 0,0,0) \\
(2)' & \quad 2' \quad (0,0,1/2) \quad 0,0,z \quad (2_z \mid 0,0,1/2)'
(3)' & \quad 2' \quad (0,1/2,0) \quad 0,y,1/4 \quad (2_y \mid 0,1/2,1/2)'
(4) & \quad 2 \quad x,1/4,0 \quad (2_z \mid 0,1/2,0) \\
(5)' & \quad \bar{1} \quad 0,0,0 \quad (1 \mid 0,0,0)'
(6) & \quad m \quad x,y,1/4 \quad (m_z \mid 0,0,1/2) \\
(7) & \quad c \quad (0,0,1/2) \quad x,1/4,z \quad (m_y \mid 0,1/2,1/2) \\
(8)' & \quad b' \quad (0,1/2,0) \quad 0,y,z \quad (m_z \mid 0,1/2,0)'
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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<tr>
<th>Multiplicity</th>
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<tr>
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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
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<td>(4) x,y+1/2,z [u,v,w]</td>
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<td>(5) x,y,z+1/2 [u,v,w]</td>
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<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td>(8) x,y+1/2,z [u,v,w]</td>
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<td>0,1/2,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,01] p2m1'  Along [1,0,0] p2mg  Along [0,1,0] p2m'm'  
\(\mathbf{a}^* = -\mathbf{b}, \quad \mathbf{b}^* = \mathbf{a}\)  
\(\mathbf{a}^* = -\mathbf{c}, \quad \mathbf{b}^* = \mathbf{b}/2\)  
\(\mathbf{a}^* = \mathbf{c}/2, \quad \mathbf{b}^* = \mathbf{a}\)  
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at $\bar{1}$ on $b12_1$;

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(1) $0,0,0$

(2) $2'$ $(0,0,1/2)$ $0,0,z$
(2$^*$) $(0,0,1/2)$

(3) 2 $(0,1/2,0)$ $0,y,1/4$
(2$^*$) $(0,1/2,1/2)$

(4) $2'$ $x,1/4,0$
(4$^*$) $(0,1/2,0)$

(5) $\bar{1}$ $0,0,0$
($\bar{1}$) $0,0,0$

(6) $m$ $x,y,1/4$
($m_z$) $(0,0,1/2)$

(7) $c'$ $(0,0,1/2)$ $x,1/4,z$
($m_y$) $(0,1/2,1/2)$

(8) $b$ $(0,1/2,0)$ $0,y,z$
($m_z$) $(0,1/2,0)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>8</th>
<th>e</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z+1/2 [u,v,w]</th>
<th>(3) x,y+1/2,z+1/2 [u,v,w]</th>
<th>(4) x,y+1/2,z [u,v,w]</th>
<th>(5) x,y,z [u,v,w]</th>
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<th>(7) x,y+1/2,z+1/2 [u,v,w]</th>
<th>(8) x,y+1/2,z [u,v,w]</th>
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<tbody>
<tr>
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<td>d</td>
<td>.m</td>
<td>x,y,1/4 [0,0,w]</td>
<td>x,y,3/4 [0,0,w]</td>
<td>x,y+1/2,1/4 [0,0,0,w]</td>
<td>x,y+1/2,3/4 [0,0,w]</td>
<td>x,y,1/4 [0,v,w]</td>
<td>x,3/4,1/2 [0,v,w]</td>
<td>x,3/4,0 [0,v,w]</td>
<td>x,1/4,1/2 [0,v,w]</td>
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<tr>
<td>4</td>
<td>c</td>
<td>2.</td>
<td>x,1/4,0 [0,v,w]</td>
<td>x,3/4,1/2 [0,v,w]</td>
<td>x,1/2,0,1/2 [0,0,0]</td>
<td>x,1/2,0,1/2 [0,0,0]</td>
<td>x,1/4,0 [0,v,w]</td>
<td>x,1/4,0 [0,v,w]</td>
<td>x,1/2,0,1/2 [0,0,0]</td>
<td>x,1/2,0,1/2 [0,0,0]</td>
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<tr>
<td>4</td>
<td>a</td>
<td>1</td>
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<td>0,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mg1'  Along [1,0,0]  p2b, 2mg  Along [0,1,0]  p2mm
a* = -b  b* = a  a* = -c  b* = b/2  a* = c/2  b* = a
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
**Origin** at \( \bar{1} \) on \( b12 \)

**Asymmetric unit**

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{4} \]

**Symmetry Operations**

1. \((1)\) \(\bar{1} \quad (0,0,0)\)
   
2. \((1)\) \(2 \quad (0,0,1/2) \quad 0,0,z\)
   
3. \((1)\) \(2' \quad (0,1/2,0) \quad 0,y,1/4\)
   
4. \((1)\) \(2' \quad x,1/4,0\)
   
5. \((5)\) \(\bar{1} \quad 0,0,0\)
   
6. \((5)\) \(m' \quad x,y,1/4\)
   
7. \((5)\) \(c \quad (0,0,1/2) \quad x,1/4,z\)
   
8. \((5)\) \(b \quad (0,1/2,0) \quad 0,y,z\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td>4 d .m'</td>
<td>x,y,1/4 [u,v,0]</td>
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<td>4 c 2'</td>
<td>x,1/4,0 [0,v,w]</td>
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<td>4 b 1'</td>
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<td>0,0,0 [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1]  p2mg  Along [1,0,0]  p2b, 2mg  Along [0,1,0]  p2a, 2mm
a* = -b  b* = a  a* = -c  b* = b/2  a* = c/2  b* = a
Origin at 0,0,z  Origin at x,1/4,0  Origin at 0,y,0
Pb’c’m

m’m’m

Orthorhombic

57.6.463

P2'/b'2,'/c'2,/m

Origin at 1 on b’12,

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
(1 0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2z 0,0,1/2)

(3) 2’ (0,1/2,0) 0,y,1/4
(2,0,1/2,1/2)’

(4) 2’ x,1/4,0
(2,0,1/2,0)’

(5) 1
(1 0,0,0)

(6) m x,y,1/4
(mz 0,0,1/2)

(7) c’ (0,0,1/2) x,1/4,z
(m,0,1/2,1/2)’

(8) b’ (0,1/2,0) 0,y,z
(m,0,1/2,0)’
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>(8) x,y+1/2,z [u,v,w]</td>
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<td>4 d ..m</td>
<td>x,y,1/4 [0,0,w]</td>
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<td>x,y,3/4 [0,0,w]</td>
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<td>x,y+1/2,3/4 [0,0,w]</td>
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<td>x,1/4,1/2 [0,v,w]</td>
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<tr>
<td>4 b 1</td>
<td>1/2,0,0 [u,v,w]</td>
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Symmetry of Special Projections

Along [0,01]  p2mg1'  Along [1,0,0]  p 2'mg'  Along [0,1,0]  p 2'mm'
\( a^* = -b \)  \( b^* = a \)  \( a^* = -c \)  \( b^* = b/2 \)  \( a^* = c/2 \)  \( b^* = a \)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Pbc'm'

mm'm'

Orthorhombic

57.7.464

P2/b2₁ /c'2₁ /m'

Origin at 0 on b12₁

Asymmetric unit

\( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

(1) \( \bar{1} \) (1 | 0,0,0)  
(2) \( 2' (0,0,1/2) \quad 0,0,z \)  
(3) \( 2' (0,1/2,0) \quad 0,y,1/4 \)  
(4) \( 2 \ x,1/4,0 \)  
(5) \( \bar{1} \) 0,0,0  
(6) \( m' \ x,y,1/4 \)  
(7) \( c' (0,0,1/2) \ x,1/4,z \)  
(8) \( b (0,1/2,0) \ 0,y,z \)

\( (2z | 0,0,1/2)' \)  
\( (2y | 0,1/2,1/2)' \)  
\( (2x | 0,1/2,0) \)  
\( (m_z | 0,0,1/2)' \)  
\( (m_y | 0,1/2,1/2)' \)  
\( (m_x | 0,1/2,0) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<td>(3) (x, y+1/2, z+1/2 [u,v,w])</td>
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<tr>
<td>4 c 2..</td>
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<td>(9) x,y,z [u,v,w]</td>
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<td>(10) x,y,1/4 [u,v,0]</td>
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<td>(16) x,3/4,0 [u,0,0]</td>
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<td>(17) x,1/4,1/2 [u,0,0]</td>
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<td>(18) 1/2,0,0 [u,v,w]</td>
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<td>(23) 0,0,1/2 [u,v,w]</td>
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<td>(24) 0,1/2,1/2 [u,v,w]</td>
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<td>(25) 0,1/2,0 [u,v,w]</td>
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</table>

### Symmetry of Special Projections

- **Along [0,01]** \(\ p2'm'g\)  \(a^* = -b\)  \(b^* = a\)  
  Origin at 0,0,z
- **Along [1,0,0]** \(\ p_{2b} \2m'g'\)  \(a^* = -c\)  \(b^* = b/2\)  
  Origin at x,1/4,0
- **Along [0,1,0]** \(\ p \ 2'mm'\)  \(a^* = -a\)  \(b^* = c/2\)  
  Origin at 0,y,0

---

57.7.464 - 2 - 919
Origin at $\bar{1}$ on $b'12_1^\prime$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $1$
   
   
   

2. $2'$ $(0,0,1/2) \quad 0,0,z$
   
   

3. $2 (0,1/2,0) \quad 0,y,1/4$
   
   

4. $2' \quad x,1/4,0$
   
   

5. $1 \quad 0,0,0$
   
   

6. $m' \quad x,y,1/4$
   
   

7. $c (0,0,1/2) \quad x,1/4,z$
   
   

8. $b' (0,1/2,0) \quad 0,y,z$
   
   

57.8.465 - Pb'cm'

57.8.465 m'm'm'

Orthorhombic

57.8.465 P2'/b'/2_1^\prime/c2_1^\prime/m'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions  
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</table>

Symmetry of Special Projections

Along [0,01]  p2'mg'  Along [1,0,0]  p 2'm'g  Along [0,1,0]  p2a',2m'm'
\( \mathbf{a}^* = -\mathbf{b} \  \mathbf{b}^* = \mathbf{a} \)  \( \mathbf{a}^* = -\mathbf{c} \  \mathbf{b}^* = \mathbf{b}/2 \)  \( \mathbf{a}^* = \mathbf{c}/2 \  \mathbf{b}^* = \mathbf{a} \)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,1/4
Origin at \( \overline{1} \) on \( b'12_1 \).

Asymmetric unit: \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/4 \)

Symmetry Operations:

1. \( 1 \) 
   \( (1 | 0,0,0) \)

2. \( 2 (0,0,1/2) 0,0,z \) 
   \( (2z | 0,0,1/2) \)

3. \( 2 (0,1/2,0) 0,y,1/4 \) 
   \( (2z | 0,1/2,1/2) \)

4. \( 2 x,1/4,0 \) 
   \( (2x | 0,1/2,0) \)

5. \( \overline{1} 0,0,0 \) 
   \( (\overline{1} | 0,0,0) \) 
   \( (m_z | 0,0,1/2) \)

6. \( m' x,y,1/4 \) 
   \( (m_z | 0,0,1/2) \)

7. \( c' (0,0,1/2) x,1/4,z \) 
   \( (m_y | 0,1/2,1/2) \)

8. \( b' (0,1/2,0) 0,y,z \) 
   \( (m_y | 0,1/2,0) \)
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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**Symmetry of Special Projections**

- Along [0,01] p2m'g'  
  - a' = -b  b' = a
  - Origin at 0,0,z

- Along [1,0,0] p 2m'g'  
  - a' = -c  b' = b/2
  - Origin at x,0,0

- Along [0,1,0] p 2m'm'  
  - a' = c/2  b' = a
  - Origin at 0,y,0
Orthorhombic

$P_{2a}$ bcm

57.10.467

$mmm'$

$P_{2a}2/b2_1/c2_1/m$

Origin at $\bar{1}$ on $b12_1$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0)$ + set

(1) $1$
(2) $2$ $(0,0,1/2)$ $0,0,z$
(3) $2'$ $(0,1/2,0)$ $0,y,1/4$
(4) $2$ $(0,1/2,0)$ $x,1/4,0$

For $(1,0,0)'$ + set

(5) $\bar{1}$ $0,0,0$
(6) $m$ $x,y,1/4$
(7) $n'$ $(0,0,1/2)$ $x,1/4,z$
(8) $b$ $(0,1/2,0)$ $0,y,z$

(1) $t'$ $(1,0,0)'
(2) 2'$ $(0,0,1/2)$ $1/2,0,z$
(3) $2'$ $(0,1/2,0)$ $1/2,y,1/4$
(4) $2'$ $(1,0,0)$ $x,1/4,0$

(5) $\bar{1}'$ $1/2,0,0$
(6) $a'$ $(1,0,0)$ $x,y,1/4$
(7) $n'$ $(1,0,1/2)$ $x,1/4,z$
(8) $b'$ $(0,1/2,0)$ $1/2,y,z$

(1) $1$
(2) $2$ $(0,0,1/2)$ $0,0,1/2$
(3) $2$ $(0,1/2,1/2)$

(5) $\bar{1}$ $0,0,0$
(6) $m$ $x,y,1/4$
(7) $n'$ $(0,0,1/2)$ $x,1/4,z$
(8) $b$ $(0,1/2,0)$ $0,y,z$

(1) $t'$ $(1,0,0)'
(2) 2'$ $(0,0,1/2)$ $1/2,0,1/2'$
(3) $2'$ $(1,1/2,1/2')$
(4) $2'$ $(1,0,0)$ $x,1/4,0$

(5) $\bar{1}'$ $1/2,0,0$
(6) $a'$ $(1,0,0)$ $x,y,1/4$
(7) $n'$ $(1,0,1/2)$ $x,1/4,z$
(8) $b'$ $(0,1/2,0)$ $1/2,y,z$

(1) $1$
(2) $2$ $(0,0,1/2)$ $0,0,1/2$
(3) $2$ $(0,1/2,1/2)$

(5) $\bar{1}$ $0,0,0$
(6) $m$ $x,y,1/4$
(7) $n'$ $(0,0,1/2)$ $x,1/4,z$
(8) $b$ $(0,1/2,0)$ $0,y,z$

(1) $t'$ $(1,0,0)'
(2) 2'$ $(0,0,1/2)$ $1/2,0,1/2'$
(3) $2'$ $(1,1/2,1/2')$
(4) $2'$ $(1,0,0)$ $x,1/4,0$

(5) $\bar{1}'$ $1/2,0,0$
(6) $a'$ $(1,0,0)$ $x,y,1/4$
(7) $n'$ $(1,0,1/2)$ $x,1/4,z$
(8) $b'$ $(0,1/2,0)$ $1/2,y,z$
Generators selected (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<thead>
<tr>
<th>Position</th>
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<th>Muliplicity</th>
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<tr>
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<td>(0,0,0) +</td>
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<tr>
<td>8 b 1'</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
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<td>0,0,0 [u,v,w]</td>
<td>0,0,1/2 [u,v,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p2mg1'   Along [1,0,0] p2mg1'   Along [0,1,0] p c 2mm
a* = -b   b* = a       a* = -c   b* = b/2       a* = c/2   b* = a
Origin at 0,0,z          Origin at x,0,0          Origin at 0,y,1/4
**Origin** at $\overline{1}b_{12}'$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

For $(0,0,0) + set$

1. $I^{(0,0,0)}$
2. $2'(0,0,1/2) \quad 0,0,z$
3. $2(0,1/2,0) \quad 0,y,1/4$
4. $2' \quad x,1/4,0$
5. $m \quad x,y,1/4$
6. $n \quad (m_{z}|0,0,1/2)$
7. $c'(0,0,1/2) \quad x,1/4,z$
8. $b \quad (0,1/2,0) \quad 0,y,z$

For $(1,0,0)' + set$

1. $I'(1,0,0)$
2. $2(0,0,1/2) \quad 1/2,0,z$
3. $2'(0,1/2,0) \quad 1/2,y,1/4$
4. $2 \quad (1,0,0) \quad x,1/4,0$
5. $a'(1,0,0) \quad x,y,1/4$
6. $n(1,0,1/2) \quad x,1/4,z$
7. $b'(0,1/2,0) \quad 1/2,y,z$
8. $m_{z}(1,0,1/2)$
**Generators selected**  (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<tr>
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<tr>
<td>(1,0,0)'</td>
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</tr>
<tr>
<td>(1,0,0)'</td>
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</table>

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<tr>
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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(4) x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
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<tr>
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<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td>(5) x,y,z</td>
<td>(8) x,y+1/2,z [u,v,w]</td>
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</table>

| 8 d       | x,y,1/4 [0,0,w]              |
|           | x,y,3/4 [0,0,w]              |
|           | x,y+1/2,1/4 [0,0,w]          |
|           | x,y+1/2,3/4 [0,0,w]          |

| 8 c       | x,1/4,0 [0,v,w]              |
|           | x,3/4,1/2 [0,v,w]            |
|           | x,3/4,0 [0,v,w]              |
|           | x,1/4,1/2 [0,v,w]            |

| 8 b       | 1/2,0,0 [u,v,w]              |
|           | 1/2,0,1/2 [u,v,w]            |
|           | 1/2,1/2,1/2 [u,v,w]          |
|           | 1/2,1/2,0 [u,v,w]            |

| 8 a       | 0,0,0 [0,0,0]                |
|           | 0,0,1/2 [0,0,0]              |
|           | 0,1/2,1/2 [0,0,0]            |
|           | 0,1/2,0 [0,0,0]              |

**Symmetry of Special Projections**

- **Along [0,01]**  
  - p2mg1'  
    - a* = -b  
    - b* = a
  - Origin at 0,0,z

- **Along [1,0,0]**  
  - p2mg1'  
    - a* = -c  
    - b* = b/2
  - Origin at x,0,0

- **Along [0,1,0]**  
  - p2a, 2mm  
    - a* = -a  
    - b* = c/2
  - Origin at 0,y,0
Origin at \( \bar{1} \) on \( b12 \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

For \((0,0,0)\) + set

1. \( 1 \)
   \((0,0,0)\)

2. \( 2 \)
   \((0,0,1/2)\) 0,0,z
   \((2_z,0,0,1/2)\)

3. \( 2' \)
   \((0,1/2,0)\) 0,y,1/4
   \((2_{z'}|0,1/2,1/2\)')

4. \( 2' \)
   \((x,1/4,0)\)
   \((2_{z'}|0,1/2,0\)')

5. \( \bar{1} \)
   \((0,0,0)\)

6. \( m' \)
   \((x,y,1/4)\)
   \((m_{z'}|0,0,1/2\)')

7. \( c \)
   \((0,0,1/2)\) x,1/4,z
   \((m_{y'}|0,1/2,1/2\)')

8. \( b \)
   \((0,1/2,0)\) 0,y,z
   \((m_{x'}|0,1/2,0\)')

For \((1,0,0)\)' + set

1. \( t' \)
   \((1,0,0)\)

2. \( 2' \)
   \((0,0,1/2)\) 1/2,0,z
   \((2_{z'}|1,0,1/2\)')

3. \( 2 \)
   \((0,1/2,0)\) 1/2,y,1/4
   \((2_{y'}|1,1/2,1/2\)')

4. \( 2 \)
   \((1,0,0)\) x,1/4,0
   \((2_{x'}|1,1/2,0\)')

5. \( \bar{1} \)
   \((1,0,0)\)

6. \( a \)
   \((1,0,0)\) x,y,1/4
   \((m_{z'}|1,0,1/2\)')

7. \( n' \)
   \((1,0,1/2)\) x,1/4,z
   \((m_{y'}|1,1/2,1/2\)')

8. \( b' \)
   \((0,1/2,0)\) 1/2,y,z
   \((m_{x'}|1,1/2,0\)')
Generators selected  (1); t'(1,0,0); t(0,0,1); t(0,0,1); (2); (3); (5).

Positions

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<td></td>
</tr>
<tr>
<td>(1,0,0)' +</td>
<td></td>
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</tbody>
</table>

16 e 1
(1) x,y,z [u,v,w]
(2) x,y,z+1/2 [u,v,w]
(3) x,y+1/2,z+1/2 [u,v,w]
(4) x,y+1/2,z [u,v,w]
(5) x,y,z [u,v,w]
(6) x,y,z+1/2 [u,v,w]
(7) x,y+1/2,z+1/2 [u,v,w]
(8) x,y+1/2,z [u,v,w]

8 d ..m' x,y,1/4 [u,v,0]
(2) x,y,3/4 [u,v,0]
(3) x,y+1/2,1/4 [u,v,0]
(4) x,y+1/2,3/4 [u,v,0]

8 c 2'.. x,1/4,0 [0,v,w]
(6) x,3/4,1/2 [0,v,w]
(7) x,3/4,0 [0,v,w]
(8) x,1/4,1/2 [0,v,w]

8 b 1/2,0,0 [u,v,w]
(1) 1/2,0,1/2 [u,v,w]
(2) 1/2,1/2,1/2 [u,v,w]
(3) 1/2,1/2,0 [u,v,w]

8 a 1' 0,0,0 [0,0,0]
(1) 0,0,1/2 [0,0,0]
(2) 0,1/2,1/2 [0,0,0]
(3) 0,1/2,0 [0,0,0]

Symmetry of Special Projections

Along [0,01]  p 2b 2mg
a* = -c  b* = a
Origin at 0,0,z

Along [1,0,0]  p 2mg1'
a* = -c  b* = b/2
Origin at x,0,0

Along [0,1,0]  p 2mm
a* = c/2  b* = a
Origin at 0,y,0
Origin at \( \bar{1} \) on \( b1\bar{2},' \)

Asymmetric unit \( 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{4} \)

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2' (0,0,1/2) \quad 0,0,z \\
(3) & \quad 2' (0,1/2,0) \quad 0,y,1/4 \\
(4) & \quad 2 \quad x,1/4,0 \\
(5) & \quad 1/2,0,0 \\
(6) & \quad m' x,y,1/4 \\
(7) & \quad c' (0,0,1/2) \quad x,1/4,z \\
(8) & \quad b (0,1/2,0) \quad 0,y,z
\end{align*}
\]

For \((1,0,0)\) + set

\[
\begin{align*}
(1) & \quad t' (1,0,0) \\
(2) & \quad 2 (0,0,1/2) \quad 1/2,0,z \\
(3) & \quad 2 (0,1/2,0) \quad 1/2,y,1/4 \\
(4) & \quad 2' (1,0,0) \quad x,1/4,0 \\
(5) & \quad 1/2,0,0 \\
(6) & \quad a (1,0,0) \quad x,y,1/4 \\
(7) & \quad n (1,0,1/2) \quad x,1/4,z \\
(8) & \quad b' (0,1/2,0) \quad 1/2,y,z
\end{align*}
\]
Generators selected  (1); t'(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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<tr>
<td>16</td>
<td>e 1</td>
<td>(1) x, y, z [u, v, w]</td>
<td>(2) x, y, z+1/2 [u, v, w]</td>
<td>(3) x, y+1/2, z+1/2 [u, v, w]</td>
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<tr>
<td></td>
<td></td>
<td>(5) x, y, z [u, v, w]</td>
<td>(6) x, y, z+1/2 [u, v, w]</td>
<td>(7) x, y+1/2, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td>8</td>
<td>d ..m'</td>
<td>x, y, 1/4 [u, v, 0]</td>
<td>x, y, 3/4 [u, v, 0]</td>
<td>x, y+1/2, 1/4 [u, v, 0]</td>
</tr>
<tr>
<td>8</td>
<td>c 2-</td>
<td>x, 1/4, 0 [u, 0, 0]</td>
<td>x, 3/4, 1/2 [u, 0, 0]</td>
<td>x, 3/4, 0 [u, 0, 0]</td>
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<tr>
<td>8</td>
<td>b 1-</td>
<td>1/2, 0, 0 [0, 0, 0]</td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
<td>1/2, 1/2, 1/2 [0, 0, 0]</td>
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<tr>
<td>8</td>
<td>a 1</td>
<td>0, 0, 0 [u, v, w]</td>
<td>0, 0, 1/2 [u, v, w]</td>
<td>0, 1/2, 1/2 [u, v, w]</td>
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Symmetry of Special Projections

Along [0, 0, 1]  \( p_{2a} \) 2m'g' \[ \begin{align*} a^* &= -b & b^* &= a \end{align*} \] Origin at 1/4, 0, z
Along [1, 0, 0]  \( p 2m1' \) \[ \begin{align*} a^* &= -c & b^* &= b/2 \end{align*} \] Origin at x, 0, 0
Along [0, 1, 0]  \( p_{2a} \) 2m'm' \[ \begin{align*} a^* &= -a & b^* &= c/2 \end{align*} \] Origin at 1/4, y, 1/4

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Origin at center (2/m)

Asymmetric unit  
0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

1. 1
   0,0,0

2. 0,0,z
   0,0,0

3. 0,0,1/2
   0,0,1/2

4. 1/2,0,0
   1/2,0,0

5. 1,0,0
   1,0,0

6. x,y,0
   0,0,0

7. x,1/4,0
   x,1/4,0

8. 1/4,1/4,0
   1/4,1/4,0

9. x,1/4,1/4
   x,1/4,1/4

10. 1/4,1/4,1/4
    1/4,1/4,1/4

11. 1/2,1/2,1/2
    1/2,1/2,1/2

12. 1/2,1/2,1/2
    1/2,1/2,1/2

13. 1/2,1/2,1/2
    1/2,1/2,1/2

14. 1/2,1/2,1/2
    1/2,1/2,1/2

15. 1/2,1/2,1/2
    1/2,1/2,1/2

16. 1/2,1/2,1/2
    1/2,1/2,1/2

17. 1/2,1/2,1/2
    1/2,1/2,1/2

18. 1/2,1/2,1/2
    1/2,1/2,1/2

19. 1/2,1/2,1/2
    1/2,1/2,1/2

20. 1/2,1/2,1/2
    1/2,1/2,1/2

21. 1/2,1/2,1/2
    1/2,1/2,1/2
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<tr>
<td>2 c ..2/m</td>
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<tr>
<td>2 b ..2/m</td>
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<tr>
<td>2 a ..2/m</td>
<td>0,0,0 [0,0,w] 1/2,1/2,1/2 [0,0,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p2gg1' a* = a b* = b
Along [1,0,0] c_p 2'mm' a* = -c b* = b
Along [0,1,0] c_p 2'mm' a* = c b* = a
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at center (2/m1')

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For 1 + set

(1) 1  
(1 | 0,0,0)

(2) 2  0,0,z  
(2 | 0,0,0)

(3) 2 (0,1/2,0) 1/4,y,1/4  
(2 | 1/2,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,1/4  
(2 | 1/2,1/2,1/2)

(5) m  0,0,0  
(m | 0,0,0)

(6) m' x,y,0  
(m' | 0,0,0)

(7) n (1/2,0,1/2) x,1/4,z  
(n | 1/2,1/2,1/2)

(8) n (0,1/2,1/2) 1/4,y,z  
(n | 1/2,1/2,1/2)

For 1' + set

(1) 1'  
(1 | 0,0,0')

(2) 2' 0,0,z  
(2 | 0,0,0')

(3) 2' (0,1/2,0) 1/4,y,1/4  
(2 | 1/2,1/2,1/2')

(4) 2' (1/2,0,0) x,1/4,1/4  
(2 | 1/2,1/2,1/2')

(5) m' 0,0,0  
(m' | 0,0,0')

(6) m' x,y,0  
(m' | 0,0,0')

(7) n' (1/2,0,1/2) x,1/4,z  
(n' | 1/2,1/2,1/2')

(8) n' (0,1/2,1/2) 1/4,y,z  
(n' | 1/2,1/2,1/2')
Continued 58.2.472 Pnnm1'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions
Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,y,z [0,0,0]</td>
<td>8</td>
<td>h</td>
<td>11'</td>
</tr>
<tr>
<td>x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td>(3)</td>
<td>(3)</td>
<td></td>
</tr>
<tr>
<td>x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td>(4)</td>
<td>(4)</td>
<td></td>
</tr>
<tr>
<td>x,y,z [0,0,0]</td>
<td>(5)</td>
<td>(5)</td>
<td></td>
</tr>
<tr>
<td>x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td>(6)</td>
<td>(6)</td>
<td></td>
</tr>
<tr>
<td>0,1/2,z [0,0,0]</td>
<td>4</td>
<td>f</td>
<td>.21'</td>
</tr>
<tr>
<td>1/2,0,z+1/2 [0,0,0]</td>
<td>(7)</td>
<td>(7)</td>
<td></td>
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<tr>
<td>1/2,0,z [0,0,0]</td>
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<td>(8)</td>
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<tr>
<td>0,0,z [0,0,0]</td>
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<td>e</td>
<td>.21'</td>
</tr>
<tr>
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<tr>
<td>1/2,1/2,z [0,0,0]</td>
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<tr>
<td>0,1/2,0 [0,0,0]</td>
<td>2</td>
<td>c</td>
<td>.2/m1'</td>
</tr>
<tr>
<td>1/2,0,1/2 [0,0,0]</td>
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<td>(11)</td>
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<tr>
<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
<td>0,0,1/2 [0,0,0]</td>
<td>2</td>
<td>b</td>
<td>.2/m1'</td>
</tr>
<tr>
<td>1/2,1/2,0 [0,0,0]</td>
<td>(13)</td>
<td>(13)</td>
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<tr>
<td>1/2,1/2,0 [0,0,0]</td>
<td>(14)</td>
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<tr>
<td>0,0,0 [0,0,0]</td>
<td>2</td>
<td>a</td>
<td>.2/m1'</td>
</tr>
<tr>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>(16)</td>
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</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2gg1'  
Along [1,0,0] c 2mm1'  
Along [0,1,0] c 2mm1'

\[ a^* = a \quad b^* = b \]  
\[ a^* = b \quad b^* = c \]  
\[ a^* = c \quad b^* = a \]  

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center (2'/$m$)

Asymmetric unit: $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/2$

Symmetry Operations:

1. $1$
   \[ (1|0,0,0) \]
2. $2'$
   \[ (2_z|0,0,0) \]
3. $2'$
   \[ (2_z|1/2,1/2,1/2) \]
4. $2$
   \[ (1/2,0,0) \]
   \[ x,1/4,1/4 \]
5. $1$
   \[ (0,0,0)' \]
6. $m$
   \[ (m_z|0,0,0) \]
7. $n$
   \[ (m_y|1/2,1/2,1/2) \]
8. $n'$
   \[ (m_z|1/2,1/2,1/2) \]
Generators selected  $(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5)$.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 h 1</td>
<td>$(1) x,y,z [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(2) \bar{x},\bar{y},\bar{z} [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(3) x+1/2,y+1/2,z+1/2 [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(4) x+1/2,y+1/2,z+1/2 [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(5) x,y,z [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(6) x,y,z [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(7) x+1/2,y+1/2,z+1/2 [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(8) x+1/2,y+1/2,z+1/2 [u,v,w]$</td>
</tr>
<tr>
<td>4 g ..m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 f ..2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z+1/2 [u,v,0]</td>
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<tr>
<td></td>
<td>0,1/2,z [u,v,0]</td>
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<td></td>
<td>1/2,0,z+1/2 [u,v,0]</td>
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<tr>
<td>4 e ..2'</td>
<td>0,0,z [u,v,0]</td>
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<tr>
<td></td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
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<td>0,0,z [u,v,0]</td>
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<tr>
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<td>1/2,1/2,z+1/2 [u,v,0]</td>
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<tr>
<td>2 d ..2'/m</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 c ..2'/m</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b ..2'/m</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2 a ..2'/m</td>
<td>0,0,0 [0,0,0]</td>
</tr>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2gg1'</th>
<th>Along [1,0,0] c2mm</th>
<th>Along [0,1,0] c_p 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = a$ $b^* = b$</td>
<td>$a^* = b$ $b^* = c$</td>
<td>$a^* = c$ $b^* = a$</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>

58.3.473 - 2 - 937
Orthorhombic

Pnnm' 58.4.474  mmm'  P2₁/n2₁/n2/m'

Origin at center (2/m')

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

<table>
<thead>
<tr>
<th>(1) 1</th>
<th>(2) 2</th>
<th>(3) 2'</th>
<th>(4) 2'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1</td>
<td>0,0,0)</td>
<td>(2z</td>
<td>0,0,0)</td>
</tr>
<tr>
<td>(5) 2'</td>
<td>(6) m'</td>
<td>(7) n</td>
<td>(8) n</td>
</tr>
<tr>
<td>0,0,0</td>
<td>x,y,0</td>
<td>(1/2,0,1/2)</td>
<td>(0,1/2,1/2)</td>
</tr>
<tr>
<td>(1</td>
<td>0,0,0)'</td>
<td>(m</td>
<td>0,0,0)'</td>
</tr>
</tbody>
</table>

Symmetry Operations

<table>
<thead>
<tr>
<th>(1) 1</th>
<th>(2) 2</th>
<th>(3) 2'</th>
<th>(4) 2'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1</td>
<td>0,0,0)</td>
<td>(2z</td>
<td>0,0,0)</td>
</tr>
<tr>
<td>(5) 2'</td>
<td>(6) m'</td>
<td>(7) n</td>
<td>(8) n</td>
</tr>
<tr>
<td>0,0,0</td>
<td>x,y,0</td>
<td>(1/2,0,1/2)</td>
<td>(0,1/2,1/2)</td>
</tr>
<tr>
<td>(1</td>
<td>0,0,0)'</td>
<td>(m</td>
<td>0,0,0)'</td>
</tr>
</tbody>
</table>
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(6) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(7) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
</tr>
</tbody>
</table>

| 4 g ..m'     | x, y, 0 [u, v, 0] |
|              | x, y, 0 [u, v, 0] |
|              | x+1/2, y+1/2, 1/2 [u, v, 0] |
|              | x+1/2, y+1/2, 1/2 [u, v, 0] |
|              | x+1/2, y+1/2, 1/2 [u, v, 0] |

| 4 f ..2      | 0, 1/2, z [0, 0, w] |
|              | 1/2, 0, z+1/2 [0, 0, w] |
|              | 0, 1/2, z [0, 0, w] |
|              | 1/2, 0, z+1/2 [0, 0, w] |

| 4 e ..2      | 0, 0, z [0, 0, w] |
|              | 1/2, 1/2, z+1/2 [0, 0, w] |
|              | 0, 0, z [0, 0, w] |
|              | 1/2, 1/2, z+1/2 [0, 0, w] |

| 2 d ..2/m'   | 0, 1/2, 1/2 [0, 0, 0] |
|              | 1/2, 0, 0 [0, 0, 0] |

| 2 c ..2/m'   | 0, 1/2, 0 [0, 0, 0] |
|              | 1/2, 0, 1/2 [0, 0, 0] |

| 2 b ..2/m'   | 0, 0, 1/2 [0, 0, 0] |
|              | 1/2, 1/2, 0 [0, 0, 0] |

| 2 a ..2/m'   | 0, 0, 0 [0, 0, 0] |
|              | 1/2, 1/2, 1/2 [0, 0, 0] |

**Symmetry of Special Projections**

Along [0,0,1]  p2gg  
Along [1,0,0]  c_p` 2m`m`

a^* = a  b^* = b  
a^* = b  b^* = c  
a^* = c  b^* = a

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
**Orthorhombic**

Pn'n'm  
58.5.475  
m'm'm  
P2₁/n'2₁/n'2/m

**Origin** at center (2/m)

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

(1) 1
(1 | 0,0,0)  
(2) 2 0,0,z
(2z | 0,0,0)

(3) 2' (0,1/2,0) 1/4,y,1/4
(2y' | 1/2,1/2,1/2)

(4) 2' (1/2,0,0) x,1/4,1/4
(2z' | 1/2,1/2,1/2)

(5) 1
(1 | 0,0,0)  
(6) m x,y,0
(mz | 0,0,0)

(7) n' (1/2,0,1/2) x,1/4,z
(my | 1/2,1/2,1/2)

(8) n' (0,1/2,1/2) 1/4,y,z
(mz | 1/2,1/2,1/2)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter, Site Symmetry</th>
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</thead>
<tbody>
<tr>
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<td>x,y,z [u,v,w]</td>
<td>1 (1)</td>
</tr>
<tr>
<td>8 h 1</td>
<td>x,y,z [u,v,w]</td>
<td>2 (1)</td>
</tr>
<tr>
<td>8 h 1</td>
<td>x,y,z [u,v,w]</td>
<td>3 (1)</td>
</tr>
<tr>
<td>8 h 1</td>
<td>x,y,z [u,v,w]</td>
<td>4 (1)</td>
</tr>
<tr>
<td>8 h 1</td>
<td>x,y,z [u,v,w]</td>
<td>5 (1)</td>
</tr>
<tr>
<td>4 g .m</td>
<td>x,y,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 f .2</td>
<td>0,1/2,2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 e .2</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 d .2/m</td>
<td>0,1/2,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 c .2/m</td>
<td>0,1/2,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b .2/m</td>
<td>0,0,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 a .2/m</td>
<td>0,0,0 [0,0,w]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2gg1'</th>
<th>Along [1,0,0] c 2'mm'</th>
<th>Along [0,1,0] c 2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = -c b* = b</td>
<td>a* = c b* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
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</tbody>
</table>
Pnn'\textit{m}'

58.6.476

Orthorhombic

\begin{align*}
\text{mm}'\textit{m}' & \quad P2_1/n2_1'/n'2'm' \\
\end{align*}

\textbf{Origin} at center (2'/m')

\textbf{Asymmetric unit} \quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2

\textbf{Symmetry Operations}

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 2', 0,0,z \\
(2) & \quad (0,0,0)' \\
(3) & \quad 2' (0,1/2,0), 1/4,y,1/4 \\
(3) & \quad (0,1/2,1/2)' \\
(4) & \quad 2 (1/2,0,0), x,1/4,1/4 \\
(4) & \quad (1/2,1/2,1/2) \\
(5) & \quad 1 \\
(5) & \quad (0,0,0) \\
(6) & \quad m', x,y,0 \\
(6) & \quad (0,0,0)' \\
(7) & \quad n' (1/2,0,1/2), x,1/4,z \\
(7) & \quad (1/2,1/2,1/2)' \\
(8) & \quad n (0,1/2,1/2), 1/4,y,z \\
(8) & \quad (1/2,1/2,1/2) \\
\end{align*}
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Site Symmetry</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 g ..m'</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
<td>x+1/2,y+1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 f ..2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>1/2,0,z+1/2 [u,v,0]</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 e ..2'</td>
<td>0,0,z [u,v,0]</td>
<td>1/2,1/2,z+1/2 [u,v,0]</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>2 d ..2'/m'</td>
<td>0,1/2,1/2 [u,v,0]</td>
<td>1/2,0,0 [u,v,0]</td>
<td>1/2,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2 c ..2'/m'</td>
<td>0,1/2,0 [u,v,0]</td>
<td>1/2,1/2,0 [u,v,0]</td>
<td>1/2,1/2,0 [u,v,0]</td>
</tr>
<tr>
<td>2 b ..2'/m'</td>
<td>0,0,1/2 [u,v,0]</td>
<td>1/2,1/2,1/2 [u,v,0]</td>
<td>1/2,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>2 a ..2'/m'</td>
<td>0,0,0 [u,v,0]</td>
<td>1/2,1/2,1/2 [u,v,0]</td>
<td>1/2,1/2,1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p2'gg' \( a^* = a \) \( b^* = b \) \( c_{2'} \) \( 2'mm' \) Along [1,0,0] c \( 2mm' \) \( a^* = b \) \( b^* = c \) \( c_2 \) \( 2mm' \) Along [0,1,0] c \( 2mm' \) \( a^* = -a \) \( b^* = c \) \( c_2 \) \( 2mm' \) Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at center (2/m')

Asymmetric unit 0 $\leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

\[
\begin{align*}
\text{(1)} & \quad 1 \\
& \quad (1|0,0,0) \\
\text{(2)} & \quad 2 \quad 0,0,z \\
& \quad (2_z|0,0,0) \\
\text{(3)} & \quad 2 \quad (0,1/2,0) \quad 1/4,y,1/4 \\
& \quad (2_z|1/2,1/2,1/2) \\
\text{(4)} & \quad 2 \quad (1/2,0,0) \quad x,1/4,1/4 \\
& \quad (2_z|1/2,1/2,1/2) \\
\text{(5)} & \quad \bar{1} \quad 0,0,0 \\
& \quad (\bar{1}|0,0,0)' \\
\text{(6)} & \quad m' \quad x,y,0 \\
& \quad (m_z|0,0,0)' \\
\text{(7)} & \quad n' \quad (1/2,0,1/2) \quad x,1/4,z \\
& \quad (m_y|1/2,1/2,1/2)' \\
\text{(8)} & \quad n' \quad (0,1/2,1/2) \quad 1/4,y,z \\
& \quad (m_y|1/2,1/2,1/2)' 
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</thead>
<tbody>
<tr>
<td>8 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

| 4 g ..m'     | x,y,0 [u,v,0] |
|              | x,y,0 [u,v,0] |
|              | x+1/2,y+1/2,1/2 [u,v,0] |

| 4 f .2       | 0,1/2,z [0,0,w] |
|              | 1/2,0,z+1/2 [0,0,w] |
|              | 0,1/2,z [0,0,w] |
|              | 1/2,0,z+1/2 [0,0,w] |

| 4 e .2       | 0,0,z [0,0,w] |
|              | 1/2,1/2,z+1/2 [0,0,w] |
|              | 0,0,z [0,0,w] |
|              | 1/2,1/2,z+1/2 [0,0,w] |

| 2 d ..2/m'   | 0,1/2,1/2 [0,0,0] |
|              | 1/2,0,0 [0,0,0] |

| 2 c ..2/m'   | 0,1/2,0 [0,0,0] |
|              | 1/2,0,1/2 [0,0,0] |

| 2 b ..2/m'   | 0,0,1/2 [0,0,0] |
|              | 1/2,1/2,0 [0,0,0] |

| 2 a ..2/m'   | 0,0,0 [0,0,0] |
|              | 1/2,1/2,1/2 [0,0,0] |

Symmetry of Special Projections

- Along [0,0,1]  p2g'g'  
  \[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  
  Origin at 0,0,z

- Along [1,0,0]  c 2m'm'  
  \[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]  
  Origin at x,0,0

- Along [0,1,0]  c 2m'm'  
  \[ \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a} \]  
  Origin at 0,y,0
Origin at mm2/n at 1/4,1/4,0 from $\overline{1}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $T$ 
   - $1$ (0,0,0)
   - $Ti$ (1/2,1/2,0)

2. $2$ 
   - $0,0,z$
   - $0,0,0$
   - $1/4,0,0$

3. $2$ 
   - $(0,1/2,0)\ 1/4,y,0$
   - $(2z,1/2,1/2,0)$

4. $2$ 
   - $(1/2,0,0)\ x,1/4,0$
   - $(2z,1/2,1/2,0)$

5. $T$ 
   - $1/4,1/4,0$
   - $1/2,1/2,0$

6. $n$ 
   - $(1/2,1/2,0)\ x,y,0$
   - $(m,z,1/2,1/2,0)$

7. $m$ 
   - $x,0,z$
   - $(0,0,0)$

8. $m$ 
   - $0,y,z$
   - $(0,0,0)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
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</table>

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<tbody>
<tr>
<td>Along [0,0,1] c_p,2mm</td>
</tr>
<tr>
<td>a* = a b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
</tr>
</tbody>
</table>

59.1.478 - 2 - 947
**Origin** at mm2/n1' at 1/4,1/4,0 from 11'

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For 1 + set

1. $I \quad (1|0,0,0)$
2. $2 \quad 0,0,z \quad (2_z|0,0,0)$
3. $2 \quad (0,1/2,0) \quad 1/4,y,0 \quad (2_y|1/2,1/2,0)$
4. $2 \quad (1/2,0,0) \quad x,1/4,0 \quad (2_x|1/2,1/2,0)$
5. $T \quad 1/4,1/4,0 \quad (1|2,1/2,0)$
6. $n \quad (1/2,1/2,0) \quad x,y,0 \quad (m_z|1/2,1/2,0)$
7. $m \quad x,0,z \quad (m_y|0,0,0)$
8. $m' \quad 0,y,z \quad (m_x|0,0,0)$

For 1' + set

1. $t' \quad (1|0,0,0)'$
2. $2' \quad 0,0,z \quad (2_z|0,0,0)'$
3. $2' \quad (0,1/2,0) \quad 1/4,y,0 \quad (2_y|1/2,1/2,0)'$
4. $2' \quad (1/2,0,0) \quad x,1/4,0 \quad (2_x|1/2,1/2,0)'$
5. $t' \quad 1/4,1/4,0 \quad (1|2,1/2,0)'$
6. $n' \quad (1/2,1/2,0) \quad x,y,0 \quad (m_z|1/2,1/2,0)'$
7. $m' \quad x,0,z \quad (m_y|0,0,0)'$
8. $m' \quad 0,y,z \quad (m_x|0,0,0)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

8 g 11'

(1) x,y,z [0,0,0]  
(2) x,y,z [0,0,0]  
(3) x+1/2,y+1/2,z [0,0,0]  
(4) x+1/2,y+1/2,z [0,0,0]  
(5) x+1/2,y+1/2,z [0,0,0]  
(6) x+1/2,y+1/2,z [0,0,0]  
(7) x,y,z [0,0,0]  
(8) x,y,z [0,0,0]

4 f .m.1’ x,0,z [0,0,0]   x,0,z [0,0,0]  
4 e m..1’ 0,y,z [0,0,0]      0,y,z [0,0,0]  
4 d 11’ 1/4,1/4,1/2 [0,0,0]      3/4,3/4,1/2 [0,0,0]  
4 c 11’ 1/4,1/4,0 [0,0,0]      3/4,3/4,0 [0,0,0]  
2 b mm21’ 0,1/2,z [0,0,0]     1/2,0,z [0,0,0]  
2 a mm21’ 0,0,z [0,0,0]       1/2,1/2,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  c2mm1’
Along [1,0,0]  p2mg1’
Along [0,1,0]  p2mg1’

\( a^* = a \quad b^* = b \)
\( a^* = b \quad b^* = c \)
\( a^* = -a \quad b^* = c \)

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at 1/4,y,0
Origin at m'm2'/n at 1/4,1/4,0 from \( \bar{1} \)

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations:

1. \( \bar{1} \)
2. \( 2' \) 0,0,z
3. \( 2' (0,1/2,0) \) 1/4,y,0
4. \( 2 (1/2,0,0) \) x,1/4,0
5. \( \bar{1} \) 1/4,1/4,0
6. \( n (1/2,1/2,0) \) x,y,0
7. \( m \) x,0,z
8. \( m' \) 0,y,z
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

8 g 1

8g 1

(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) x+1/2,y+1/2,z [u,v,w]  (4) x+1/2,y+1/2,z [u,v,w]
(5) x+1/2,y+1/2,z [u,v,w]  (6) x+1/2,y+1/2,z [u,v,w]  (7) x,y,z [u,v,w]  (8) x,y,z [u,v,w]

4 f .m. x,0,z [0,v,0]  x,0,z [0,v,0]  x+1/2,1/2,z [0,v,0]  x+1/2,1/2,z [0,v,0]
4 e m'. 0,y,z [0,v,w]  0,y,z [0,v,w]  1/2,y+1/2,z [0,v,w]  1/2,y+1/2,z [0,v,w]
4 d 1 1/4,1/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]
4 c 1 1/4,1/4,0 [0,0,0]  3/4,3/4,0 [0,0,0]  1/4,3/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]
2 b m'm2' 0,1/2,z [0,v,0]  1/2,0,z [0,v,0]
2 a m'm2' 0,0,z [0,v,0]  1/2,1/2,z [0,v,0]

Symmetry of Special Projections

Along [0,0,1] cₚₚ2'mm'  Along [1,0,0] p2mg  Along [0,1,0] p2mg1'
a* = -b  b* = a  a* = b  b* = c  a* = -a  b* = c
Origin at 0,0,z  Origin at x,1/4,0  Origin at 1/4,y,0
Origin at mm2/n' at 1/4,1/4,0 from $\overline{1}$

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$

Symmetry Operations

(1) $\overline{1}$
(2) $2\overline{2}$ 0,0,z
(3) $2'$ (0,1/2,0) 1/4,y,0
(4) $2'$ (1/2,0,0) x,1/4,0
(5) $\overline{1}$ 1/4,1/4,0
(6) $n'$ (1/2,1/2,0) x,y,0
(7) $m$ x,0,z
(8) $m$ 0,y,z

Orthorhombic

Pmmn' mmn' 59.4.481
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
<td>(8) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 f .m.</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
<td>x+1/2,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>4 e m..</td>
<td>0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
<td>1/2,y+1/2,z [u,0,0]</td>
</tr>
<tr>
<td>4 d 1</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,3/4,1/2 [0,0,0]</td>
<td>1/4,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c 1</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,3/4,0 [0,0,0]</td>
<td>1/4,3/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b mm2</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a mm2</td>
<td>0,0,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
<td></td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2mm  Along [1,0,0]  p2mg1'  Along [0,1,0]  p2mg1'
\(a^* = a\)  \(b^* = b\)  \(a^* = b\)  \(b^* = c\)  \(a^* = -a\)  \(b^* = c\)
Origin at 0,0,z  Origin at x,1/4,0  Origin at 1/4,y,0
Orthorhombic

Origin at m'm'2/n at 1/4,1/4,0 from \( \bar{1} \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. \( 1 \)
   
   \[
   \begin{align*}
   (1) & \quad 1 \\
   (1 | 0,0,0) & \\
   \end{align*}
   \]

2. \( 2 \)
   
   \[
   \begin{align*}
   (2) & \quad 0,0,z \\
   (2z | 0,0,0) & \\
   \end{align*}
   \]

3. \( 2' \)
   
   \[
   \begin{align*}
   (3) & \quad (0,1/2,0) \quad 1/4,0,0 \quad (2,|1/2,1/2,0) \\
   & \quad (2z | 1/2,1/2,0)' & \quad (2,|1/2,1/2,0)' \\
   \end{align*}
   \]

4. \( 2' \)
   
   \[
   \begin{align*}
   (4) & \quad (1/2,0,0) \quad x,1/4,0 \\
   & \quad (2,|1/2,1/2,0) & \quad (2,|1/2,1/2,0)' \\
   \end{align*}
   \]

5. \( \bar{1} \)
   
   \[
   \begin{align*}
   (5) & \quad 1/4,1/4,0 \\
   (1 | 1/2,1/2,0) & \\
   \end{align*}
   \]

6. \( n \)
   
   \[
   \begin{align*}
   (6) & \quad (1/2,1/2,0) \quad x,y,0 \\
   & \quad (mz | 1/2,1/2,0) \\
   \end{align*}
   \]

7. \( m' \)
   
   \[
   \begin{align*}
   (7) & \quad m',x,0,z \\
   & \quad (m | 0,0,0)' \\
   \end{align*}
   \]

8. \( m' \)
   
   \[
   \begin{align*}
   (8) & \quad m',0,y,z \\
   & \quad (m | 0,0,0)' \\
   \end{align*}
   \]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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(1) x,y,z [u,v,w]  
(2) x+1/2,y+1/2,z [u,v,w]  
(3) x+1/2,y+1/2,z [u,v,w]  
(4) x+1/2,y+1/2,z [u,v,w]  

(5) x+1/2,y+1/2,z [u,v,w]  
(6) x+1/2,y+1/2,z [u,v,w]  
(7) x,y,z [u,v,w]  
(8) x,y,z [u,v,w]

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<tr>
<td>Along [0,0,1] c_p 2m' m'</td>
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<tr>
<td>a* = a  b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
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</table>
Origin at mm'2'/n' at 1/4,1/4,0 from \( \bar{1} \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

1. \( \bar{1} \) (1 0,0,0) \( \bar{1} \) (1 0,0,0)
2. \( 2' \) 0,0,z 0,0,0')
3. \( 2' (0,1/2,0) 1/4,y,0 (2z,1/2,1/2,0) \)
4. \( 2 (1/2,0,0) x,1/4,0 (2z,1/2,1/2,0) \)
5. \( \bar{1} 1/4,1/4,0 (1/2,1/2,0) \)
6. \( n' (1/2,1/2,0) x,y,0 (m_z,1/2,1/2,0)' \)
7. \( m' x,0,z (m_y,0,0,0)' \)
8. \( m 0,y,z (m_z,0,0,0) \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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Symmetry of Special Projections

<table>
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<tr>
<th>Along [0,0,1]</th>
<th>c2'mm'</th>
<th>Along [1,0,0]</th>
<th>p2mg1'</th>
<th>Along [0,1,0]</th>
<th>p2'mg'</th>
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<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,1/4,0</td>
<td></td>
<td>Origin at 1/4,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at $m'm'2/n'$ at $1/4,1/4,0$ from $\overline{1}'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $1 (1|0,0,0)$
2. $2 (0,0,z)$  
   $(2_z|0,0,0)$
3. $2 (0,1/2,0) \quad 1/4,y,0$  
   $(2_{y,1/2,1/2,0})$
4. $2 (1/2,0,0) \quad x,1/4,0$  
   $(2_z|1/2,1/2,0)$
5. $\overline{1}' \quad 1/4,1/4,0$  
   $(\overline{1} | 1/2,1/2,0)'$
6. $n' (1/2,1/2,0) \quad x,y,0$  
   $(m_z|1/2,1/2,0)'$
7. $m' \quad x,0,z$  
   $(m_y|0,0,0)'$
8. $m' \quad 0,y,z$  
   $(m_z|0,0,0)'$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td></td>
</tr>
<tr>
<td>4 f .m.'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>4 e m'.</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 d .1</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c .1</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b m'm2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a m'm2</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,1/4,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -a</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 1/4,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at mm2/n at 1/4,1/4,0 from \( \overline{1} \)

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \)  
   \((1|0,0,0)\)

2. \(2\)  
   \((0,0,z)\)  
   \((2_z|0,0,0)\)

3. \(2\)  
   \((0,1/2,0)\)  
   \((1/4,y,0)\)  
   \((2_y|1/2,1/2,0)\)

4. \(2\)  
   \((1/2,0,0)\)  
   \((x,1/4,0)\)  
   \((2_x|1/2,1/2,0)\)

5. \(\overline{1}\)  
   \((1/4,1/4,0)\)  
   \((1/2,1/2,0)\)

6. \(n\)  
   \((1/2,1/2,2,0)\)  
   \((x,y,0)\)  
   \((m_2|1/2,1/2,0)\)

7. \(m\)  
   \((x,0,z)\)  
   \((m_y|0,0,0)\)

8. \(m\)  
   \((0,y,z)\)  
   \((m_x|0,0,0)\)

For \((0,0,1) + \) set

1. \(t'\)  
   \((0,0,1)\)  
   \((1|0,0,1)\)

2. \(2'\)  
   \((0,0,1)\)  
   \((0,0,z)\)  
   \((2_z|0,0,1)'\)

3. \(2'\)  
   \((0,1/2,0)\)  
   \((1/4,y,1/2)\)  
   \((2_y|1/2,1/2,1)'\)

4. \(2'\)  
   \((1/2,0,0)\)  
   \((x,1/4,1/2)\)  
   \((2_x|1/2,1/2,1)'\)

5. \(\overline{1}\)  
   \((1/4,1/4,1/2)\)  
   \((1/2,1/2,1)'\)

6. \(n'\)  
   \((1/2,1/2,2,0)\)  
   \((x,y,1/2)\)  
   \((m_2|1/2,1/2,1)'\)

7. \(c'\)  
   \((0,0,1)\)  
   \((x,0,z)\)  
   \((m_y|0,0,1)'\)

8. \(c'\)  
   \((0,0,1)\)  
   \((0,y,z)\)  
   \((m_x|0,0,1)'\)
Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td>(0,0,0) + (0,0,1)</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x',y',z' [u',v',w']</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+1/2,y+1/2,z' [u',v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x+1/2,y'+1/2,z' [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x+1/2,y+1/2,z' [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x+1/2,y+1/2,z' [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f.m.</td>
<td>x,0,z [0,v,0]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 e.m.</td>
<td>0,y,z [u,0,0]</td>
<td>(2) x',y',z' [u',v',w']</td>
</tr>
<tr>
<td>8 d 1'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>(3) x+1/2,y+1/2,z' [u',v,w]</td>
</tr>
<tr>
<td>8 c 1</td>
<td>1/4,1/4,0 [u,v,w]</td>
<td>(4) x+1/2,y'+1/2,z' [u,v,w]</td>
</tr>
<tr>
<td>4 b mm2</td>
<td>0,1/2,z [0,0,0]</td>
<td>(5) x+1/2,y+1/2,z' [u,v,w]</td>
</tr>
<tr>
<td>4 a mm2</td>
<td>0,0,z [0,0,0]</td>
<td>(6) x+1/2,y+1/2,z' [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1' a* = a  b* = b
Along [1,0,0] p2mg1' a* = b  b* = c
Along [0,1,0] p2mg1' a* = -a  b* = c

Origin at 0,0,z Origin at x,1/4,0 Origin at 1/4,y,0
Origin at m’m2’/n at 1/4,1/4,0 from \( \overline{T} \)

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \quad (1|0,0,0)\)
2. \(2' \quad 0,0,z\) \( (2_z|0,0,0)' \)
3. \(2' \quad (0,1/2,0) \quad 1/4,y,0\) \( (2_z|1/2,1/2,0)' \)
4. \(2 \quad (1/2,0,0) \quad x,1/4,0\) \( (2_z|1/2,1/2,0) \)
5. \(\overline{T} \quad 1/4,1/4,0\)
6. \((\overline{T}|1/2,1/2,0)' \)
7. \(m \quad x,0,z\) \( (m_z|0,0,0) \)
8. \(m' \quad 0,y,z\) \( (m_z|0,0,0)' \)

For \((0,0,1)' + \) set

1. \(t' \quad (0,0,1)\)
2. \((1,0,0)' \)
3. \(2 \quad (0,1/2,0) \quad 1/4,y,1/2\) \( (2_z|1/2,1/2,1) \)
4. \(2' \quad (1/2,0,0) \quad x,1/4,1/2\) \( (2_z|1/2,1/2,1)' \)
5. \(\overline{T} \quad 1/4,1/4,1/2\)
6. \((\overline{T}|1/2,1/2,1)' \)
7. \(c' \quad (0,0,1) \quad x,0,z\) \( (m_z|0,0,0)' \)
8. \(c \quad (0,0,1) \quad 0,y,z\) \( (m_z|0,0,1) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity,</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>Wyckoff letter,</td>
<td>(0,0,1)' +</td>
</tr>
<tr>
<td>Site Symmetry.</td>
<td>(0,0,0) +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x ,y ,z [u,v,w]</th>
<th>(3) x+1/2,y+1/2,z [u,v,w]</th>
<th>(4) x+1/2,y+1/2,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16 g</td>
<td>x,y,z [u,v,w]</td>
<td></td>
<td>x+1/2,1/2,1/2 [0,v,w]</td>
<td>x+1/2,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>(5) x+1/2,y+1/2,z</td>
<td>1/2,y+1/2,z [0,v,w]</td>
<td>1/2,y+1/2,z [0,v,w]</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td>(6) x+1/2,y+1/2,z</td>
<td>1/2,y+1/2,z [0,v,w]</td>
<td>1/2,y+1/2,z [0,v,w]</td>
</tr>
<tr>
<td>1/2</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>4</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c2mm1'</th>
<th>Along [1,0,0] p2mg</th>
<th>Along [0,1,0] p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = -a b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 1/4,y,0</td>
</tr>
</tbody>
</table>
Origin at m'm'2/n at 1/4,1/4,0 from m

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1 0,0,0
1 0,0,0
1/4,1/4,0
1/2,1/2,0

1/4,1/4,1/2
1/2,1/2,1/2

(1) 1
(2) 2 0,0,z
(2) 0,0,0
(3) 2' (0,1/2,0) 1/4,y,0
(2) 1/2,1/2,0)
(4) 2' (1/2,0,0) x,1/4,0
(2) 1/2,1/2,0)

(5) 1/4,1/4,0
(6) n (1/2,1/2,0) x,y,0
(6) 1/2,1/2,0)
(7) m' x,0,z
(7) 0,0,0')
(8) m' 0,y,z
(8) 0,0,0')

For (0,0,1) + set

1 0,0,1
1 0,0,1
1/4,1/4,1/2
1/2,1/2,1/2

x,y,0
x,0,z
x,0,z
x,0,z

(1) t' (0,0,1)
(2) 2' (0,0,1) 0,0,z
(2) 0,0,1')
(3) 2 (0,1/2,0) 1/4,y,1/2
(3) 1/2,1/2,1)
(4) 2 (1/2,0,0) x,1/4,1/2
(4) 1/2,1/2,1)

(5) 1/4,1/4,1/2
(6) n' (1/2,1/2,0) x,y,1/2
(6) 1/2,1/2,1)
(7) c (0,0,1) x,0,z
(7) 0,0,1)
(8) c (0,0,1) 0,y,z
(8) 0,0,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

<table>
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<tr>
<th>Positions</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(0,0,0) + (0,0,1) +</td>
</tr>
<tr>
<td>16 g 1</td>
<td></td>
</tr>
<tr>
<td>(1) (x,y,z [u,v,w])</td>
<td>(2) (x,y,z, [u,v,w])</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>(5) (x+1/2, y+1/2, z [u,v,w])</td>
<td>(6) (x+1/2, y+1/2, z [u,v,w])</td>
</tr>
<tr>
<td>8 f .m'.</td>
<td>(x,0,z [u,0,w])</td>
</tr>
<tr>
<td>8 e m'.</td>
<td>(0,y,z [0,v,w])</td>
</tr>
<tr>
<td>8 d ( \bar{T} )</td>
<td>(1/4,1/4,1/2 [0,0,0])</td>
</tr>
<tr>
<td>8 c ( \bar{T} )</td>
<td>(1/4,1/4,0 [u,v,w])</td>
</tr>
<tr>
<td>4 b m'm'2</td>
<td>(0,1/2,z [0,0,w])</td>
</tr>
<tr>
<td>4 a m'm'2</td>
<td>(0,0,z [0,0,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c2mm1'</th>
<th>Along [1,0,0] p2m'g'</th>
<th>Along [0,1,0] p2v, 2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a) (b^* = b)</td>
<td>(a^* = b) (b^* = c)</td>
<td>(a^* = -a) (b^* = c)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,1/4</td>
<td>Origin at 1/4,y,0</td>
</tr>
</tbody>
</table>
Origin at $\bar{1}$ on 1c1

Asymmetric unit: $0 \leq x < 1/2$; $0 \leq y < 1/2$; $0 \leq z \leq 1/2$

Symmetry Operations:

1. $1$  
   $(1 | 0,0,0)$

2. $2$ (0,0,1/2)  
   $1/4,1/4,z$  
   $(2 | 1/2,1/2,1/2)$

3. $2$  
   $0,y,1/4$  
   $(2 | 0,0,1/2)$

4. $2$ (1/2,0,0)  
   $x,1/4,0$  
   $(2 | 1/2,1/2,0)$

5. $\bar{1}$  
   $(1 | 0,0,0)$

6. $n$ (1/2,1/2,0)  
   $x,y,1/4$  
   $(m_2 | 1/2,1/2,1/2)$

7. $c$ (0,0,1/2)  
   $x,0,z$  
   $(m_y | 0,0,1/2)$

8. $b$ (0,1/2,0)  
   $1/4,y,z$  
   $(m_z | 1/2,1/2,0)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 8 d 1        | (1) x,y,z [u,v,w]  
                | (2) x+1/2,y+1/2,z+1/2 [u,v,w]  
                | (3) x,y,z+1/2 [u,v,w]  
                | (4) x+1/2,y+1/2,z [u,v,w]  
                | (5) x,y,z [u,v,w]  
                | (6) x+1/2,y+1/2,z+1/2 [u,v,w]  
                | (7) x,y,z+1/2 [u,v,w]  
                | (8) x+1/2,y+1/2,z [u,v,w] |
| 4 c .2.      | 0,y,1/4 [0,v,0]  
                | 1/2,y+1/2,3/4 [0,v,0]  
                | 0,y,3/4 [0,v,0]  
                | 1/2,y+1/2,1/4 [0,v,0] |
| 4 b 1        | 0,1/2,0 [u,v,w]  
                | 1/2,0,1/2 [u,v,w]  
                | 0,1/2,1/2 [u,v,w]  
                | 1/2,0,0 [u,v,w] |
| 4 a 1        | 0,0,0 [u,v,w]  
                | 1/2,1/2,1/2 [u,v,w]  
                | 0,0,1/2 [u,v,w]  
                | 1/2,1/2,0 [u,v,w] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] c_p 2'mm'</th>
<th>Along [1,0,0] p_{2b}. 2m'g'</th>
<th>Along [0,1,0] p_{2b}. 2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = -b  b' = a</td>
<td>a' = -c  b' = b/2</td>
<td>a' = -a  b' = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Pbcn1'  
$60.2.489$

mmm1'  
$P2_1/b2/c2\overline{1}/n1'$

Orthorhombic

Origin at $\bar{1}1'$ on $1c11'$

Asymmetric unit  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $1'$ set

- $1'$, $(1' | 0,0,0)$
- $2'$, $(0,0,1/2)$, $1/4,1/4,z$
- $2'$, $(1/2,0,0)$, $x,1/4,0$
- $3'$, $(0,0,1/2)$, $x,0,z$
- $4'$, $(0,1/2,0)$, $1/4,y,z$

For $1' + set$

- $(1 | 0,0,0)$
- $(2 | 0,0,1/2)$, $1/4,1/4,z$
- $(2 | 1/2,1/2,1/2)$
- $(3 | 0,0,1/2)$, $x,0,z$
- $(4 | 0,0,1/2)$, $x,1/4,0$

- $(5 | 0,0,0)$
- $(6 | 1/2,1/2,0)$, $x,1/4$
- $(7 | 0,0,1/2)$, $y,1/4$
- $(8 | 1/2,1/2,0)$, $1/4,y,z$

- $(1' | 0,0,0)$
- $(2' | 0,0,1/2)$, $1/4,1/4,z$
- $(2' | 1/2,1/2,1/2)$
- $(3' | 0,0,1/2)$, $x,0,z$
- $(4' | 1/2,0,0)$, $x,1/4,0$

- $(5' | 0,0,0)$
- $(6' | 1/2,1/2,0)$, $x,1/4$
- $(7' | 0,0,1/2)$, $x,0,z$
- $(8' | 0,1/2,0)$, $1/4,y,z$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>8</td>
<td>(2) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td>1</td>
</tr>
<tr>
<td>(3) x,y,z+1/2 [0,0,0]</td>
<td></td>
<td>(4) x+1/2,y+1/2,z-</td>
<td>1' +</td>
</tr>
<tr>
<td>(5) x,y,z-</td>
<td></td>
<td>[0,0,0]</td>
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<tr>
<td>(6) x+1/2,y+1/2,z+1/2</td>
<td>(7) x,y,z+1/2 [0,0,0]</td>
<td>(8) x+1/2,y+1/2,z</td>
<td>[0,0,0]</td>
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<tr>
<td>(8) x+1/2,y+1/2,z</td>
<td></td>
<td>[0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1'  
Along [1,0,0] p 2mg1'  
Along [0,1,0] p 2mg1'

a* = a  b* = b  c* = b/2  
a* = -a  b* = c/2  c* = c/2

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at \( \bar{1} \) on 1c1

Asymmetric unit: \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations:

1. \( 1 \) \( (0,0,0) \)
2. \( 2' (0,0,1/2) \) \( 1/4,1/4,1/2 \) \( (2\,z,1/2,1/2,1/2)' \)
3. \( 2' \) \( 0,0,1/4 \) \( (2,0,0,1/2)' \)
4. \( 2 \) \( (1/2,0,0) \) \( x,1/4,0 \) \( (2,1/2,1/2,0) \)
5. \( \bar{1} \) \( (0,0,0) \)
6. \( n (1/2,1/2,0) \) \( x,y,1/4 \) \( (m,1/2,1/2,1/2) \)
7. \( c (0,0,1/2) \) \( x,0,z \) \( (m_y,0,1/2) \)
8. \( b' (0,1/2,0) \) \( 1/4,y,z \) \( (m_z,1/2,1/2,0)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th></th>
<th>Coordinates</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .2′</td>
<td>0,y,1/4 [u,0,w]</td>
<td>1/2,y+1/2,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
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<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_{p,2mm}  Along [1,0,0] p 2mg  Along [0,1,0] p_{2b}, 2m′g′  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  \[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \]  \[ \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2 \]  
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
**Origin at \( \overline{1} \) on 1c'1**

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

1. \( \bar{1} \)
   - \( (1\bar{1}|0,0,0) \)
   - \( (1\bar{1}|0,0,0)' \)

2. \( 2' \)
   - \( (0,0,1/2) \)
   - \( (1/2,1/2,1/2)' \)

3. \( 2 \)
   - \( (0,y,1/4) \)
   - \( (2,z|0,0,1/2) \)

4. \( 2' \)
   - \( (1/2,0,0) \)
   - \( (x,1/4,0) \)

5. \( \bar{1} \)
   - \( (0,0,0) \)
   - \( (1/2,1/2,1/2)' \)

6. \( n \)
   - \( (1/2,1/2,0) \)
   - \( (x,y,1/4) \)
   - \( (m_z|1/2,1/2,1/2) \)

7. \( c' \)
   - \( (0,0,1/2) \)
   - \( (x,0,z) \)
   - \( (m_y|0,0,1/2)' \)

8. \( b \)
   - \( (0,1/2,0) \)
   - \( (1/4,y,z) \)
   - \( (m_z|1/2,1/2,0) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>(1) x,y,z [u,v,w] (2) x+1/2,y+1/2,z+1/2 [u,v,w] (3) x,y,z+1/2 [u,v,w] (4) x+1/2,y+1/2,z [u,v,w] (5) x,y,z [u,v,w] (6) x+1/2,y+1/2,z+1/2 [u,v,w] (7) x,y,z+1/2 [u,v,w] (8) x+1/2,y+1/2,z [u,v,w]</td>
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Symmetry of Special Projections

<table>
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<tr>
<th>Symmetry</th>
<th>Special Projections</th>
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<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>c_p 2m'm'</td>
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<tr>
<td>a^* = a</td>
<td>b^* = b</td>
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<tr>
<td>Origin at 0,0,z</td>
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<tr>
<td>Along [1,0,0]</td>
<td>p_4b 2m'g'</td>
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<tr>
<td>a^* = -c</td>
<td>b^* = b/2</td>
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<tr>
<td>Origin at x,0,0</td>
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<tr>
<td>Along [0,1,0]</td>
<td>p 2mg</td>
</tr>
<tr>
<td>a^* = -a</td>
<td>b^* = c/2</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
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</tbody>
</table>
Origin at $\bar{1}$ on $1c1$

Asymmetric unit \[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. $1 (0,0,0)$
2. $2 (0,0,1/2) \quad 1/4,1/4,z$
3. $2' \quad 0,y,1/4$
4. $2' (1/2,0,0) \quad x,1/4,0$
5. $\bar{1} (0,0,0)$
6. $n' (1/2,1/2,2,0) \quad x,y,1/4$
7. $c (0,0,1/2) \quad x,0,z$
8. $b (0,1/2,0) \quad 1/4,y,z$

Orthorhombic

Pbcn' 60.5.492

mmm' 60.5.492 /b2'/c2'/n'
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(3) x,y,z+1/2 [u,v,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<td>(7) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td>Along [0,0,1] c2mm</td>
</tr>
<tr>
<td>Along [1,0,0] p2b, 2mg</td>
</tr>
<tr>
<td>Along [0,1,0] p2b, 2mg</td>
</tr>
<tr>
<td>a^* = a b^* = b</td>
</tr>
<tr>
<td>a^* = -c b^* = b/2</td>
</tr>
<tr>
<td>a^* = -a b^* = c/2</td>
</tr>
</tbody>
</table>

60.5.492 - 2 - 975
Pb'c'n
60.6.493

m'm'm
P2₁/b'2'/c'2/, n

Orthorhombic

Origin at 1 on 1c'1

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2z | 1/2,1/2,1/2)

(3) 2' 0,y,1/4
(2y | 0,0,1/2)'

(4) 2' (1/2,0,0) x,1/4,0
(2x | 1/2,1/2,0)'

(5) 1
(1 | 0,0,0)

(6) n (1/2,1/2,0) x,y,1/4
(mz | 1/2,1/2,1/2)

(7) c' (0,0,1/2) x,0,z
(my | 0,0,1/2)'

(8) b' (0,1/2,0) 1/4,y,z
(mz | 1/2,1/2,0)'
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

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<td>(2) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(3) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y+1/2,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y+1/2,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
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<tr>
<td></td>
<td>1/2,1/2,0 [u,v,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c, 2mm'  Along [1,0,0] p 2'mg'  Along [0,1,0] p 2'mg
a' = a  b' = b  a' = -c  b' = b/2  a' = -a  b' = c/2
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at 1 on 1c'1

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
   (1 | 0,0,0)

(2) 2' (0,0,1/2) 1/4,1/4,z
   (2 | 1/2,1/2,1/2)'

(3) 2' 0,y,1/4
   (2 | 0,0,1/2)'

(4) 2 (1/2,0,0) x,1/4,0
   (2 | 1/2,1/2,0)

(5) 1
   (1 | 0,0,0)

(6) n' (1/2,1/2,0) x,y,1/4
   (m z | 1/2,1/2,1/2)'

(7) c' (0,0,1/2) x,0,z
   (m y | 0,0,1/2)'

(8) b (0,1/2,0) 1/4,y,z
   (m z | 1/2,1/2,0)
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5). \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 ( d ) 1 ( (1) \ x,y,z [u,v,w] ) ( (2) \ x+1/2,y+1/2,z+1/2 [u,v,w] ) ( (3) \ x,y,z+1/2 [u,v,w] ) ( (4) \ x+1/2,y+1/2,z [u,v,w] ) ( (5) \ x,y,z [u,v,w] ) ( (6) \ x+1/2,y+1/2,z+1/2 [u,v,w] ) ( (7) \ x,y,z+1/2 [u,v,w] ) ( (8) \ x+1/2,y+1/2,z [u,v,w] )</td>
<td></td>
</tr>
<tr>
<td>4 ( c ) .2' ( 0,y,1/4 [u,0,w] ) ( 1/2,y+1/2,3/4 [u,0,w] ) ( 0,y,3/4 [u,0,w] ) ( 1/2,y+1/2,1/4 [u,0,w] )</td>
<td></td>
</tr>
<tr>
<td>4 ( b ) ( 1 ) ( 0,1/2,0 [u,v,w] ) ( 1/2,0,1/2 [u,v,w] ) ( 0,1/2,1/2 [u,v,w] ) ( 1/2,0,0 [u,v,w] )</td>
<td></td>
</tr>
<tr>
<td>4 ( a ) ( \overline{1} ) ( 0,0,0 [u,v,w] ) ( 1/2,1/2,1/2 [u,v,w] ) ( 0,0,1/2 [u,v,w] ) ( 1/2,1/2,0 [u,v,w] )</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along \([0,0,1]\)**  \( c'2\text{mm}' \)
  - \( a^* = a \) \( b^* = b \)
  - Origin at \( 0,0,z \)

- **Along \([1,0,0]\)**  \( p_{2a}, 2\text{mg} \)
  - \( a^* = -c \) \( b^* = b/2 \)
  - Origin at \( x,1/4,0 \)

- **Along \([0,1,0]\)**  \( p \ 2'\text{mg}' \)
  - \( a^* = a \) \( b^* = c/2 \)
  - Origin at \( 0,y,0 \)
Pb'cn'  
60.8.495

m'mm'  
P2₁/b'/b'2/c₂, '/n'

Origin at 11 on 1c1

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) T  
(1 0,0,0)

(2) 2' (0,0,1/2) 1/4,1/4,z  
(2_{z} 1/2,1/2,1/2')

(3) 2 0,y,1/4  
(2_{y} 0,0,1/2)

(4) 2' (1/2,0,0) x,1/4,0  
(2_{x} 1/2,1,2,0')

(5) T  
(1 0,0,0)

(6) n' (1/2,1/2,0) x,y,1/4  
(m_{z} 1/2,1/2,1/2')

(7) c (0,0,1/2) x,0,z  
(m_{y} 0,0,1/2)

(8) b' (0,1/2,0) 1/4,y,z  
(m_{x} 1/2,1/2,0')
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

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<tr>
<td>4 c .2</td>
<td>0,y,1/4 [0,v,0] 1/2,y+1/2,3/4 [0,v,0] 0,y,3/4 [0,v,0] 1/2,y+1/2,1/4 [0,v,0]</td>
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<tr>
<td>4 b 1</td>
<td>0,1/2,0 [u,v,w] 1/2,0,1/2 [u,v,w] 0,1/2,1/2 [u,v,w] 1/2,0,0 [u,v,w]</td>
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<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w] 1/2,1/2,1/2 [u,v,w] 0,0,1/2 [u,v,w] 1/2,1/2,0 [u,v,w]</td>
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Symmetry of Special Projections

Along [0,0,1] c2' mm'  Along [1,0,0] p 2'm'g  Along [0,1,0] p2v, 2m'g'  
\( a^* = -b, b^* = a \)  \( a^* = -c, b^* = b/2 \)  \( a^* = -a, b^* = c/2 \)  
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
**Orthorhombic**

\[ \text{Pb}'c'n' \]

\[ \text{m}'m'm' \]

60.9.496

\[ \text{P}2_1/b'2/c'2/n' \]

**Origin** at \( \overline{1} \) on \( 1c'1 \)

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

1. \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)
2. \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)
3. \( \frac{3}{2}, \frac{3}{2}, \frac{1}{2} \)
4. \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)
5. 0, 0, 0
6. 0, 0, 0
7. 0, 0, 0
8. 0, 0, 0

\( \overline{1} \)

\( \overline{1} \)

\( \overline{1} \)

\( \overline{1} \)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

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Symmetry of Special Projections

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<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p 2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p 2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -a</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Pbca

Orthorhombic

61.1.497

mmm

P2₁/b2₁/c2₁/a

Origin at \( \overline{1} \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

\[
\begin{align*}
(1) \ & \begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix} \\
(1) \ & \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(5) \ & \begin{pmatrix} \overline{1} \\ 0,0,0 \end{pmatrix} \\
(1) \ & \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(2) \ & \begin{pmatrix} 2 \ 0,0,1/2 \end{pmatrix} \ 1/4,0,z \\
(2) \ & \begin{pmatrix} 2 \ 1/2,0,1/2 \end{pmatrix} \\
(6) \ & \begin{pmatrix} a \ 1/2,0,0 \end{pmatrix} \ x,y,1/4 \\
(6) \ & \begin{pmatrix} m_z \ 1/2,0,1/2 \end{pmatrix} \\
(3) \ & \begin{pmatrix} 2 \ 0,1/2,0 \end{pmatrix} \ 0,y,1/4 \\
(2) \ & \begin{pmatrix} 2 \ 0,1/2,1/2 \end{pmatrix} \\
(7) \ & \begin{pmatrix} c \ 0,0,1/2 \end{pmatrix} \ x,1/4,z \\
(7) \ & \begin{pmatrix} m_y \ 0,1/2,1/2 \end{pmatrix} \\
(4) \ & \begin{pmatrix} 2 \ 1/2,0,0 \end{pmatrix} \ x,1/4,0 \\
(4) \ & \begin{pmatrix} 2 \ 1/2,1/2,0 \end{pmatrix} \\
(8) \ & \begin{pmatrix} b \ 0,1/2,0 \end{pmatrix} \ 1/4,y,z \\
(8) \ & \begin{pmatrix} m_x \ 1/2,1/2,0 \end{pmatrix}
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 b 1</td>
<td>0,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**  
  $a^* = -b$  
  $b^* = a/2$  
  Origin at $1/4,0,z$

- **Along [1,0,0]**  
  $a^* = -c$  
  $b^* = b/2$  
  Origin at $x,1/4,0$

- **Along [0,1,0]**  
  $a^* = -a$  
  $b^* = c/2$  
  Origin at $0,y,1/4$
Origin at 1'1'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For 1 + set

(1) 1  
(1 | 0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z  
(2z | 1/2,0,1/2)

(3) 2 (0,1/2,0) 0,y,1/4  
(2y | 0,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0  
(2x | 1/2,1/2,0)

(5) 1  
(0,0,0)

(6) a (1/2,0,0) x,y,1/4  
(mz | 1/2,0,1/2)

(7) c (0,0,1/2) x,1/4,z  
(my | 0,1/2,1/2)

(8) b (0,1/2,0) 1/4,y,z  
(mx | 1/2,1/2,0)

For 1' + set

(1) 1'  
(1 | 0,0,0')

(2) 2' (0,0,1/2) 1/4,0,z  
(2z | 1/2,0,1/2')

(3) 2' (0,1/2,0) 0,y,1/4  
(2y | 0,1/2,1/2')

(4) 2' (1/2,0,0) x,1/4,0  
(2x | 1/2,1/2,0')

(5) 1'  
(0,0,0')

(6) a' (1/2,0,0) x,y,1/4  
(mz | 1/2,0,1/2')

(7) c' (0,0,1/2) x,1/4,z  
(my | 0,1/2,1/2')

(8) b' (0,1/2,0) 1/4,y,z  
(mx | 1/2,1/2,0)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry, Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
<td></td>
</tr>
<tr>
<td>8 c 11'</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(2) x+1/2,y,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(3) x+1/2,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(4) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(5) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(6) x+1/2,y,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(7) x,y+1/2,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(8) x,y+1/2,z+1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p 2mg1'</th>
<th>Along [1,0,0]</th>
<th>p 2mg1'</th>
<th>Along [0,1,0]</th>
<th>p 2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a/2</td>
<td>a* = -c</td>
<td>b* = b/2</td>
<td>a* = -a</td>
<td>b* = c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
Origin at x,0,0
Origin at 0,y,0
Pb’ca
61.3.499
Orthorhombic

m′mm
P2₁/b’2₁/c’2₁/a

Origin at \( \overline{1} \)

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

(1) 1
\[ (1 \mid 0,0,0) \]

(2) \( \overline{1} \)
\[ (0,0,1/2) \]
\[ 1/4,0,z \]

(3) \( \overline{2} \)
\[ (0,1/2,0) \]
\[ 0,y,1/4 \]

(4) \( \overline{2} \)
\[ (1/2,0,0) \]
\[ x,1/4,0 \]

(5) \( \overline{1} \)
\[ (0,0,0) \]

(6) \( \overline{1} \)
\[ (1/2,0,0) \]
\[ x,y,1/4 \]

(7) \( \overline{1} \)
\[ (0,0,1/2) \]
\[ x,1/4,z \]

(8) \( \overline{1} \)
\[ (0,1/2,0) \]
\[ 1/4,y,z \]
Continued 61.3.499 Pb'ca

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 4 b 1        | 0,0,1/2 [0,0,0] |
|              | 1/2,0,0 [0,0,0] |
|              | 0,1/2,0 [0,0,0] |
|              | 1/2,1/2,1/2 [0,0,0] |

| 4 a 1        | 0,0,0 [0,0,0] |
|              | 1/2,0,1/2 [0,0,0] |
|              | 0,1/2,1/2 [0,0,0] |
|              | 1/2,1/2,0 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p2 2mg
a* = -b  b* = a/2
Origin at 0,0,z

Along [1,0,0] p 2mg
a* = -c  b* = b/2
Origin at x,0,0

Along [0,1,0] p2 2m'g'
a* = -a  b* = c/2
Origin at 0,y,0
Origin at \( \bar{1} \)

Asymmetric unit: \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/2 \)

Symmetry Operations:

1. \( (1 \bar{0} 0,0,0) \)
2. \( 2 (0,0,1/2) \ 1/4,0,z \)
   \( (2z, 1/2,0,1/2) \)
3. \( 2' (0,1/2,0) \ 0,y,1/4 \)
   \( (2y, 0,1/2,1/2)' \)
4. \( 2' (1/2,0,0) \ x,1/4,0 \)
   \( (2x, 1/2,1/2,0)' \)
5. \( (5 \bar{1} 0,0,0) \)
6. \( a (1/2,0,0) \ x,y,1/4 \)
   \( (mz, 1/2,0,1/2) \)
7. \( c' (0,0,1/2) \ x,1/4,z \)
   \( (my, 0,1/2,1/2)' \)
8. \( b' (0,1/2,0) \ 1/4,y,z \)
   \( (mz, 1/2,1/2,0)' \)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinate</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 4 b 1        | 0,0,1/2 [u,v,w] | 1/2,0,0 [u,v,w] | 0,1/2,0 [u,v,w] | 1/2,1/2,1/2 [u,v,w] |
| 4 a 1        | 0,0,0 [u,v,w] | 1/2,0,1/2 [u,v,w] | 0,1/2,1/2 [u,v,w] | 1/2,1/2,0 [u,v,w] |

Symmetry of Special Projections

Along [0,0,1] p 2m'g' Along [1,0,0] p 2'mg' Along [0,1,0] p 2'm'g

\( \mathbf{a}^* = -\mathbf{b} \quad \mathbf{b}^* = \mathbf{a}/2 \) \( \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \) \( \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2 \)

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $1$
2. $(0,0,1/2) \quad 1/4,0,z$
3. $(0,1/2,0) \quad 0,y,1/4$
4. $(1/2,0,0) \quad x,1/4,0$

5. $\bar{1}$
6. $(1/2,0,0) \quad x,y,1/4$
7. $(0,0,1/2) \quad x,1/4,z$
8. $(0,1/2,0) \quad 1/4,y,z$

$Pb'c'a'$

$m'm'm'$

Orthorhombic

$P2_1/b'2_1/c'2_1/a'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8  c 1</td>
<td>(1) x,y,z [u,v,w]  (2) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2, z+1/2 [u,v,w]  (4) x+1/2, y+1/2, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]  (6) x+1/2, y+1/2, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y+1/2, z+1/2 [u,v,w]  (8) x+1/2, y+1/2, z [u,v,w]</td>
</tr>
</tbody>
</table>

4  b  1'      0,0,1/2 [0,0,0]  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]

4  a  1'      0,0,0 [0,0,0]  1/2,0,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p 2m'g'  Along [1,0,0] p 2m'g'  Along [0,1,0] p 2m'g'

\( \mathbf{a}^* = -\mathbf{b} \quad \mathbf{b}^* = \mathbf{a}/2 \)  \( \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)  \( \mathbf{a}^* = -\mathbf{a} \quad \mathbf{b}^* = \mathbf{c}/2 \)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin at $\bar{1}$ on 12,1

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) $1$
   
   (1 | 0,0,0)  

(2) $2$
   
   (0,0,1/2)  
   $1/4,0,z$
   
   $2_z | 1/2,0,1/2$

(3) $2$
   
   (0,1/2,0)  
   $0,y,0$
   
   $2_y | 0,1/2,0$

(4) $2$
   
   (1/2,0,0)  
   $x,1/4,1/4$
   
   $2_x | 1/2,1/2,1/2$

(5) $\bar{1}$
   
   (0,0,0)  

(6) $a$
   
   (1/2,0,0)  
   $x,y,1/4$
   
   $(m_z | 1/2,0,1/2)$

(7) $m$
   
   $x,1/4,z$
   
   $(m_y | 0,1/2,0)$

(8) $n$
   
   (0,1/2,1/2)  
   $1/4,y,z$
   
   $(m_x | 1/2,1/2,1/2)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,  Wyckoff letter,  Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]  (2) x+1/2,y,z+1/2 [u,v,w]  (3) x,y+1/2,z [u,v,w]  (4) x+1/2,y+1/2,z+1/2 [u,v,w]  (5) x,y,z [u,v,w]  (6) x+1/2,y+1/2,z+1/2 [u,v,w]  (7) x,y+1/2,z [u,v,w]  (8) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,1/4,z [0,v,0]  x+1/2,3/4,z+1/2 [0,v,0]  x,3/4,z [0,v,0]  x+1/2,1/4,z+1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 b    1</td>
<td>0,0,1/2 [u,v,w]  1/2,0,0 [u,v,w]  0,1/2,1/2 [u,v,w]  1/2,1/2,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a    1</td>
<td>0,0,0 [u,v,w]  1/2,0,1/2 [u,v,w]  0,1/2,0 [u,v,w]  1/2,1/2,1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p 2bb 2mg  Along [1,0,0] c p 2mm  Along [0,1,0] p 2g 1'  
\( a^* = -b \quad b^* = a/2 \) \( a^* = b \quad b^* = c \) \( a^* = c \quad b^* = a \)  
Origin at 1/4,0,z  Origin at x,1/4,1/4  Origin at 0,y,0
Origin at \(1'\) on 12;11'

Asymmetric unit: 0 ≤ \(x\) ≤ 1/2; 0 ≤ \(y\) ≤ 1/4; 0 ≤ \(z\) ≤ 1

Symmetry Operations

For 1 + set

1. (1 | 0,0,0)
2. (2 | 0,0,1/2) 1/4,0,z
3. (2 | 0,1/2,0) 0,y,0
4. (2 | 1/2,0,0) x,1/4,1/4
5. (1 | 0,0,0)'
6. (6 | a | 1/2,0,0) x,y,1/4
7. (7 | m | x,1/4,z)
8. (8 | n | 0,1/2,1/2) 1/4,y,z

For 1' + set

1. (1' | 0,0,0)'
2. (2' | 0,0,1/2) 1/4,0,z
3. (2' | 0,1/2,0) 0,y,0
4. (2' | 1/2,0,0) x,1/4,1/4
5. (1' | 0,0,0)''
6. (6' | a' | 1/2,0,0) x,y,1/4
7. (7' | m' | x,1/4,z)
8. (8' | n' | 0,1/2,1/2) 1/4,y,z

\(62.2.503\) - 1 - 996
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>d</td>
<td>11'</td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>[0,0,0]</td>
<td>(2) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(3) x,y+1/2,z</td>
<td>[0,0,0]</td>
<td>(4) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td>[0,0,0]</td>
<td>(6) x+1/2,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(7) x,y+1/2,z</td>
<td>[0,0,0]</td>
<td>(8) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>.m.1'</td>
</tr>
<tr>
<td>(1) x,1/4,z</td>
<td>[0,0,0]</td>
<td>(2) x+1/2,3/4,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(3) x,3/4,z</td>
<td>[0,0,0]</td>
<td>(4) x+1/2,1/4,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>11'</td>
</tr>
<tr>
<td>(0,0,1/2)</td>
<td>[0,0,0]</td>
<td>(1/2,0,0) [0,0,0]</td>
</tr>
<tr>
<td>(0,1/2,1/2)</td>
<td>[0,0,0]</td>
<td>(1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>11'</td>
</tr>
<tr>
<td>(0,0,0)</td>
<td>[0,0,0]</td>
<td>(1/2,0,1/2) [0,0,0]</td>
</tr>
<tr>
<td>(0,1/2,0)</td>
<td>[0,0,0]</td>
<td>(1/2,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p 2mg1' a* = -b b* = a/2
Along [1,0,0] c 2mm1' a* = b b* = c
Along [0,1,0] p 2gg1' a* = c b* = a
Origin at 0,0,z
Origin at x,1/4,1/4
Origin at 0,y,0
**Pn'ra**

62.3.504

Origin at \( \overline{1} \) on 121

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1 \]

Symmetry Operations

1. \( \overline{1} \)
2. \( 2' \) (0,0,1/2) 1/4,0,z
3. \( 2' \) (0,1/2,0) 0,y,0
4. \( 2' \) (1/2,0,0) x,1/4,1/4
5. \( \overline{1} \)
6. a (1/2,0,0) x,y,1/4
7. m x,1/4,z
8. n' (0,1/2,1/2) 1/4,y,z

\[ (2')_{1/2,0,1/2} \]

\[ (2')_{0,1/2,0} \]

\[ (2')_{1/2,1/2,1/2} \]

\[ (m_x)_{1/2,0,1/2} \]

\[ (m_y)_{0,1/2,0} \]

\[ (m_z)_{1/2,1/2,1/2} \]
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w] (2) x+1/2,y,z+1/2 [u,v,w] (3) x,y+1/2,z [u,v,w] (4) x+1/2,y+1/2,z+1/2 [u,v,w] (5) x,y,z [u,v,w] (6) x+1/2,y,z+1/2 [u,v,w] (7) x,y+1/2,z [u,v,w] (8) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,1/4,z [0,v,0] x+1/2,3/4,z+1/2 [0,0,0] x,3/4,z [0,v,0] x+1/2,1/4,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b 1'</td>
<td>0,0,1/2 [0,0,0] 1/2,0,0 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a 1'</td>
<td>0,0,0 [0,0,0] 1/2,0,1/2 [0,0,0] 0,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2_{2}2mg

\( a^{*} = -b \quad b^{*} = a/2 \)

Origin at 0,0,z

Along [1,0,0] c 2mm

\( a^{*} = b \quad b^{*} = c \)

Origin at x,1/4,1/4

Along [0,1,0] p2gg1'

\( a^{*} = c \quad b^{*} = a \)

Origin at 0,y,0
Origin at \( \overline{1} \) on 12_1

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \]

Symmetry Operations

1. \( T \quad 0,0,0 \)
   \( (T | 0,0,0) \)
2. \( 2' (0,0,1/2) \quad 1/4,0,z \)
   \( (2_z | 1/2,0,1/2)' \)
3. \( 2 (0,1/2,0) \quad 0,y,0 \)
   \( (2_y | 0,1/2,0) \)
4. \( 2' (1/2,0,0) \quad x,1/4,1/4 \)
   \( (2_x | 1/2,1/2,1/2)' \)
5. \( \bar{T} \quad 0,0,0 \)
   \( (\bar{T} | 0,0,0)' \)
6. \( a (1/2,0,0) \quad x,y,1/4 \)
   \( (m_z | 1/2,0,1/2) \)
7. \( m' \quad x,1/4,z \)
   \( (m_y | 0,1/2,0)' \)
8. \( n (0,1/2,1/2) \quad 1/4,y,z \)
   \( (m_x | 1/2,1/2,1/2) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(2) x + 1/2, y, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(3) x, y + 1/2, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(4) x + 1/2, y + 1/2, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(6) x + 1/2, y, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(7) x, y + 1/2, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(8) x + 1/2, y + 1/2, z + 1/2 [u, v, w]</td>
</tr>
</tbody>
</table>

| 4 c .m' | x, 1/4, z [u, 0, w] |
|         | x + 1/2, 3/4, z + 1/2 [u, 0, w] |
|         | x, 3/4, z [u, 0, w] |
|         | x + 1/2, 1/4, z + 1/2 [u, 0, w] |

| 4 b ̅1' | 0, 0, 1/2 [0, 0, 0] |
|         | 1/2, 0, 0 [0, 0, 0] |
|         | 0, 1/2, 1/2 [0, 0, 0] |
|         | 1/2, 1/2, 0 [0, 0, 0] |

| 4 a ̅1' | 0, 0, 0 [0, 0, 0] |
|         | 1/2, 0, 1/2 [0, 0, 0] |
|         | 0, 1/2, 0 [0, 0, 0] |
|         | 1/2, 1/2, 1/2 [0, 0, 0] |

## Symmetry of Special Projections

Along [0, 0, 1]  p_2\text{y}. 2m'g'  
\[ \mathbf{a}^* = -\mathbf{b} \quad \mathbf{b}^* = a/2 \]

Origin at 0, 0, z

Along [1, 0, 0]  c_p. 2'mm'  
\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \]

Origin at x, 1/4, 1/4

Along [0, 1, 0]  p 2gg  
\[ \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{a} \]

Origin at 0, y, 0
Origin at $\bar{1}$ on $12\bar{1}1$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) $1$
   $(1 \mid 0,0,0)$
   
(5) $\bar{1}$
   $0,0,0$
   $(\bar{1} \mid 0,0,0)'$

(2) $2$ $(0,0,1/2)$ $1/4,0,z$
   $(2_z \mid 1/2,0,1/2)$

(6) $a'$ $(1/2,0,0)$ $x,y,1/4$
   $(m_z \mid 1/2,0,1/2)'$

(3) $2'$ $(0,1/2,0)$ $0,y,0$
   $(2_y \mid 0,1/2,0)'$

(7) $m$ $x,1/4,z$
   $(m_y \mid 0,1/2,0)$

(4) $2'$ $(1/2,0,0)$ $x,1/4,1/4$
   $(2_x \mid 1/2,1/2,1/2)'$

(8) $n$ $(0,1/2,1/2)$ $1/4,y,z$
   $(m_x \mid 1/2,1/2,1/2)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>x,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>4 b 1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p 2mg  Along [1,0,0]  c_p, 2'mm'  Along [0,1,0]  p 2gg1'
a* = -b  b* = a/2  a* = b  b* = c  a* = c  b* = a
Origin at 0,0,z  Origin at x,1/4,1/4  Origin at 0,y,0
**Origin** at \( \overline{1} \) on 12,1

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

1. \( \overline{1} \) \( \overline{1} \) \( 0,0,0 \)
2. \( (0,0,1/2) \) \( (0,1/2,0) \) \( (1/2,0,0) \)
3. \( (0,0,1/2) \) \( (0,1/2,0) \) \( (1/2,0,0) \)
4. \( (1/2,0,0) \) \( x,1/4,1/4 \)
5. \( (0,0,0) \) \( (0,1/2,0) \) \( (1/2,0,0) \)
6. \( (0,1/2,0) \) \( x,y,1/4 \)
7. \( (0,1/2,0) \) \( (1,0,1/2) \)
8. \( (0,1/2,0) \) \( (1,0,1/2) \)

**Pn'm'a**

Origin on 12,1

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \]

Symmetry Operations

1. \( \overline{1} \) \( \overline{1} \) \( 0,0,0 \)
2. \( (0,0,1/2) \) \( (0,1/2,0) \) \( (1/2,0,0) \)
3. \( (0,0,1/2) \) \( (0,1/2,0) \) \( (1/2,0,0) \)
4. \( (1/2,0,0) \) \( x,1/4,1/4 \)
5. \( (0,0,0) \) \( (0,1/2,0) \) \( (1/2,0,0) \)
6. \( (0,1/2,0) \) \( x,y,1/4 \)
7. \( (0,1/2,0) \) \( (1,0,1/2) \)
8. \( (0,1/2,0) \) \( (1,0,1/2) \)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 c .m'</td>
<td>x,1/4,z [u,0,w]</td>
<td>x+1/2,3/4,z+1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,0,1/2 [u,v,w]</td>
<td>1/2,0,0 [u,v,w]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [u,v,w]</td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  
P_{2b}, 2m'g'  
\[ a^* = -b \quad b^* = a/2 \]  
Origin at 0,0,z

Along [1,0,0]  
c 2'm'm'  
\[ a^* = -c \quad b^* = b \]  
Origin at x,1/4,1/4

Along [0,1,0]  
p 2'gg'  
\[ a^* = c \quad b^* = a \]  
Origin at 0,y,0
Origin at \( \frac{1}{2}, \frac{1}{2}, 0 \)

Asymmetric unit \( 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1 \)

Symmetry Operations

1. \( \overline{1} \) (1, 0, 0)
   \( (1, 0, 0) \)

2. \( 2' (0, 0, \frac{1}{2}), 1/4, 0, z \)
   \( (2, \frac{1}{2}, 0, \frac{1}{2})' \)

3. \( 2' (0, 1/2, 0) \) \( 0, y, 0 \)
   \( (2, \frac{1}{2}, 0, \frac{1}{2})' \)

4. \( 2 (1/2, 0, 0) \) \( x, 1/4, 1/4 \)
   \( (2, \frac{1}{2}, 1/2, 1/2) \)

5. \( \overline{1} (0, 0, 0) \)
   \( (1, 0, 0) \)

6. \( a' (1/2, 0, 0), x, y, 1/4 \)
   \( (m, 1/2, 0, 1/2)' \)

7. \( m' x, 1/4, z \)
   \( (m, 1/2, 0, 1/2)' \)

8. \( n (0, 1/2, 1/2) \) \( 1/4, y, z \)
   \( (m, 1/2, 1/2)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) (x,y,z) ([u,v,w]) ( (2) \ \bar{x}+1/2,\bar{y},z+1/2) ([u,v,w]) ( (3) \ \bar{x},y+1/2,\bar{z}) ([u,v,w]) ( (4) x+1/2,y+1/2,\bar{z}+1/2) ([u,v,w]) ( (5) \ x,\bar{y},z) ([u,v,w]) ( (6) \ x+1/2,y,\bar{z}+1/2) ([u,v,w]) ( (7) \ x,\bar{y}+1/2,\bar{z}) ([u,v,w]) ( (8) \ \bar{x}+1/2,y+1/2,z+1/2) ([u,v,w])</td>
</tr>
<tr>
<td>4 c .m'</td>
<td>(x,1/4,z) ([u,0,w]) ( (2) \ \bar{x}+1/2,3/4,z+1/2) ([u,0,w]) ( (3) \ \bar{x},3/4,\bar{z}) ([u,0,w]) ( (4) x+1/2,1/4,\bar{z}+1/2) ([u,0,w])</td>
</tr>
<tr>
<td>4 b 1</td>
<td>(0,0,1/2) ([u,v,w]) ( (1) \ 0,1/2) ([u,v,w]) ( (2) \ 1/2,0,1/2) ([u,v,w]) ( (3) \ 0,1/2,0) ([u,v,w]) ( (4) \ 1/2,1/2,0) ([u,v,w])</td>
</tr>
<tr>
<td>4 a 1</td>
<td>(0,0,0) ([u,v,w]) ( (1) \ 1/2,0,1/2) ([u,v,w]) ( (2) \ 0,1/2,0) ([u,v,w]) ( (3) \ 1/2,1/2,1/2) ([u,v,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \( p \ 2'm'g \) Along \([1,0,0]\) \( c_p, \ 2m'm' \) Along \([0,1,0]\) \( p \ 2'gg' \)
\(a^* = -b \quad b^* = a/2\) \(a^* = b \quad b^* = c\) \(a^* = -a \quad b^* = c\)
Origin at \(0,0,z\) Origin at \(x,1/4,1/4\) Origin at \(0,y,0\)
Origin at $\bar{1}$ on 12,1

Asymmetric unit  $0 \leq x \leq 1/2;  \quad 0 \leq y \leq 1/4;  \quad 0 \leq z \leq 1$

Symmetry Operations

(1) $\bar{1}$ (0,0,0)  (2) $2' \; (0,0,1/2) \; 1/4,0,z$  (3) $2 \; (0,1/2,0) \; 0,y,0$  (4) $2' \; (1/2,0,0) \; x,1/4,1/4$

(5) $\bar{1}$ 0,0,0  (6) $a' \; (1/2,0,0) \; x,y,1/4$  (7) $m \; x,1/4,z$  (8) $n' \; (0,1/2,1/2) \; 1/4,y,z$

Origin at $\bar{1}$ on 12,1

Asymmetric unit  $0 \leq x \leq 1/2;  \quad 0 \leq y \leq 1/4;  \quad 0 \leq z \leq 1$

Symmetry Operations

(1) $\bar{1}$ (0,0,0)  (2) $2' \; (0,0,1/2) \; 1/4,0,z$  (3) $2 \; (0,1/2,0) \; 0,y,0$  (4) $2' \; (1/2,0,0) \; x,1/4,1/4$

(5) $\bar{1}$ 0,0,0  (6) $a' \; (1/2,0,0) \; x,y,1/4$  (7) $m \; x,1/4,z$  (8) $n' \; (0,1/2,1/2) \; 1/4,y,z$

62.8.509 - 1 - 1008
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5)\).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>((1) \ x, y, z [u, v, w] ) (\text{Wyckoff letter} \ x, y+1/2, z+1/2 [u, v, w] ) (\text{Wyckoff letter} \ x+1/2, y+1/2, z+1/2 [u, v, w] ) (\text{Wyckoff letter} \ x, y, z+1/2 [u, v, w] ) (\text{Wyckoff letter} \ x+1/2, y, z+1/2 [u, v, w] )</td>
</tr>
<tr>
<td>4 c .m.</td>
<td>(x, 1/4, z [0, v, 0] ) (x+1/2, 3/4, z+1/2 [0, v, 0] ) (x, 3/4, z [0, v, 0] ) (x+1/2, 1/4, z+1/2 [0, v, 0] )</td>
</tr>
<tr>
<td>4 b 1</td>
<td>(0, 0, 1/2 [u, v, w] ) (1/2, 0, 0 [u, v, w] ) (0, 1/2, 1/2 [u, v, w] ) (1/2, 1/2, 0 [u, v, w] )</td>
</tr>
<tr>
<td>4 a 1</td>
<td>(0, 0, 0 [u, v, w] ) (1/2, 0, 1/2 [u, v, w] ) (0, 1/2, 0 [u, v, w] ) (1/2, 1/2, 1/2 [u, v, w] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along \([0,0,1]\) \(p \ 2'mg'\) \(a^* = -b^* = a/2\) \(\text{Origin at } 0,0,z\)  
- Along \([1,0,0]\) \(c \ 2'mm'\) \(a^* = b^* = c\) \(\text{Origin at } x,1/4,1/4\)  
- Along \([0,1,0]\) \(p \ 2gg1'\) \(a^* = c^* \ b^* = a\) \(\text{Origin at } 0, y, 0\)
Pn'm'a'  
Origin at 1 on 12,1  
Asymmetric unit  
Symmetry Operations

\[
\begin{align*}
\text{(1) } & \quad 1 \\
& \quad (1 | 0,0,0) \\
\text{(2) } & \quad 2 (0,0,1/2) \\
& \quad (2 | 1/2,0,1/2) \\
\text{(3) } & \quad 2 (0,1/2,0) \\
& \quad (2 | 0,1/2,0) \\
\text{(4) } & \quad 2 (1/2,0,0) \\
& \quad (2 | 1/2,1/2,1/2) \\
\text{(5) } & \quad \overline{1} \\
& \quad (0,0,0) \\
& \quad (0,0,0)' \\
\text{(6) } & \quad a' (1/2,0,0) \\
& \quad (m_z | 1/2,0,1/2)' \\
\text{(7) } & \quad m' x,1/4,z \\
& \quad (m_y | 0,1/2,0)' \\
\text{(8) } & \quad n' (0,1/2,1/2) \\
& \quad (m_z | 1/2,1/2,1/2)' \\
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2, y, z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(3) x, y+1/2, z [u,v,w]</td>
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<td>(4) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
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<tr>
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<td>(6) x+1/2, y, z+1/2 [u,v,w]</td>
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<td>(7) x, y+1/2, z [u,v,w]</td>
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<td>(8) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
</tr>
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<td>x, 1/4, z [u,0,w]</td>
</tr>
<tr>
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<td>x+1/2, 3/4, z+1/2 [u,0,w]</td>
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<td>x, 3/4, z [u,0,w]</td>
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<td>1/2, 0, 0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p 2m'g'  
Along [1,0,0] c_p 2m'm'  
Along [0,1,0] p 2g'g'

\[ \mathbf{a}^* = -\mathbf{b}, \quad \mathbf{b}^* = \mathbf{a}/2 \]

Origin at 0,0,z  
Origin at 0,y,0
Origin at (2/m) at 2/mc2,

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(5) T
(1 | 0,0,0)

(2) 2 (0,0,1/2) 0,0,2m
(2 | 0,0,1/2)

(6) m x,y,1/4
(mz | 0,0,1/2)

(7) c (0,0,1/2) x,0,z
(mz | 0,0,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,2,0)
(1 | 1/2,1/2,2,0)

(5) T
(1 | 1/2,1/2,2,0)

(2) 2 (0,0,1/2) 1/4,1/4,0
(2 | 1/2,1/2,1/2)

(6) n (1/2,1/2,2,0) x,1/4
(mz | 1/2,1/2,1/2)

(7) n (1/2,0,1/2) x,1/4,0
(mz | 1/2,1/2,1/2)

(8) b (0,1/2,0) 1/4,0,1/4
(mz | 1/2,1/2,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
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<tbody>
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<td>16 h 1</td>
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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>(3) x,y,z+1/2 [u,v,w]</td>
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<td>(4) x,y,z [u,v,w]</td>
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<td>8 g ..m</td>
<td>(5) x,y,z [u,v,w]</td>
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<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td>(7) x,y,z+1/2 [u,v,w]</td>
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<td>(8) x,y,z [u,v,w]</td>
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<tr>
<td>8 f m..</td>
<td>(9) x,y,1/4 [0,0,w]</td>
</tr>
<tr>
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<td>(10) x,y,3/4 [0,0,w]</td>
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<td>(11) x,y,1/4 [0,0,w]</td>
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<td>8 e 2..</td>
<td>(12) x,0,0 [u,0,0]</td>
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<td>(13) x,0,1/2 [u,0,0]</td>
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<td>(15) x,0,1/2 [u,0,0]</td>
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<td>8 d 1</td>
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<td>(17) 3/4,3/4,1/2 [u,v,w]</td>
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<td>(21) 0,y,3/4 [0,0,0]</td>
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<td>4 b 2/m..</td>
<td>(22) 0,1/2,0 [u,0,0]</td>
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<td>(23) 0,1/2,1/2 [u,0,0]</td>
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<td>4 a 2/m..</td>
<td>(24) 0,0,0 [u,0,0]</td>
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<td>(25) 0,0,1/2 [u,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] c2mm1'  Along [1,0,0] p2mg1'  Along [0,1,0] p2a, 2mm
\[ a^* = a \quad b^* = b \]
\[ a^* = -c \quad b^* = b/2 \]
\[ a^* = c/2 \quad b^* = a/2 \]
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,1/4
Orthorhombic

Cmcm1' 63.2.512

Origin at (2/m1') at 2/mc2,1'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1  (1|0,0,0)
(2) 2 (0,0,1/2) 0,0,z (2z|0,0,1/2)
(3) 2' 0,y,1/4 (2y|0,0,1/2)
(4) 2' x,0,0 (2x|0,0,0)

(5) T 0,0,0  (T|0,0,0)
(6) m x,y,1/4 (mz|0,0,1/2)
(7) c (0,0,1/2) x,0,z (m|0,0,1/2)
(8) m 0,y,z (m|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  (1|1/2,1/2,0)
(2) 2 (0,0,1/2) 1/4,1/4,z (2z|1/2,1/2,1/2)
(3) 2 (0,1/2,0) 1/4,y,1/4 (2y|1/2,1/2,1/2)
(4) 2 (1/2,0,0) x,1/4,0 (2x|1/2,1/2,0)

(5) T 1/4,1/4,0  (1|1/2,1/2,0)
(6) n (1/2,1/2,0) x,y,1/4 (mz|1/2,1/2,1/2)
(7) n (1/2,0,1/2) x,1/4,z (m|1/2,1/2,1/2)
(8) b (0,1/2,0) 1/4,y,z (m|1/2,1/2,0)

For (0,0,0)' + set

(1) 1' (0,0,0')  (1|0,0,0')
(2) 2' (0,0,1/2) 0,0,z (2z|0,0,1/2')
(3) 2' 0,y,1/4 (2y|0,0,1/2')
(4) 2' x,0,0 (2x|0,0,0')

(5) T' 0,0,0 (T|0,0,0')
(6) m' x,y,1/4 (mz|0,0,1/2')
(7) c' (0,0,1/2) x,0,z (m|0,0,1/2')
(8) m' 0,y,z (m|0,0,0')

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0) (1|1/2,1/2,0')
(2) 2' (0,0,1/2) 1/4,1/4,z (2z|1/2,1/2,1/2')
(3) 2' (0,1/2,0) 1/4,y,1/4 (2y|1/2,1/2,1/2')
(4) 2' (1/2,0,0) x,1/4,0 (2x|1/2,1/2,0')

(5) T' 1/4,1/4,0 (1|1/2,1/2,0')
(6) n' (1/2,1/2,0) x,y,1/4 (mz|1/2,1/2,1/2')
(7) n' (1/2,0,1/2) x,1/4,z (m|1/2,1/2,1/2')
(8) b' (0,1/2,0) 1/4,y,z (m|1/2,1/2,0')
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5); 1'.

Positions

<table>
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<tr>
<th>Multiplicity</th>
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<tbody>
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<tr>
<td>Coordinates</td>
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<tr>
<td>Multiplicity</td>
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<tr>
<td>Wyckoff letter,</td>
<td></td>
</tr>
<tr>
<td>Site Symmetry.</td>
<td></td>
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</tbody>
</table>

16 h 11' (1) x,y,z [0,0,0] (2) x,y,z+1/2 [0,0,0] (3) x,y,z+1/2 [0,0,0] (4) x,y,z+1/2 [0,0,0] (5) x,y,z [0,0,0] (6) x,y,z+1/2 [0,0,0] (7) x,y,z+1/2 [0,0,0] (8) x,y,z [0,0,0]

8 g .m1' x,y,1/4 [0,0,0] x,y,3/4 [0,0,0] x,y,1/4 [0,0,0] x,y,3/4 [0,0,0]

8 f m..1' 0,y,z [0,0,0] 0,y,z+1/2 [0,0,0] 0,y,z+1/2 [0,0,0] 0,y,z [0,0,0]

8 e 2..1' x,0,0 [0,0,0] x,0,1/2 [0,0,0] x,0,1/2 [0,0,0] x,0,1/2 [0,0,0]

8 d 11' 1/4,1/4,0 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 1/4,3/4,0 [0,0,0]

4 c m2m1' 0,y,1/4 [0,0,0] 0,y,3/4 [0,0,0]

4 b 2/m..1' 0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0]

4 a 2/m..1' 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,0,0] p2mg1' Along [0,1,0] p2mm1'

\( a^* = a \) \( b^* = b \)

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at (2/m') at 2/m'c21'

Asymmetric unit

\[0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{4}\]

Symmetry Operations

For (0,0,0) + set

(1) \( \overline{1} \)
    \( (1|0,0,0) \)

(2) \( 2' \)
    \( (0,0,1/2) \)
    \( 0,0,z \)
    \( (2_z|0,0,1/2)' \)

(3) \( 2' \)
    \( 0,y,1/4 \)
    \( (2_y|0,0,1/2)' \)

(4) \( 2 \)
    \( x,0,0 \)
    \( (2_x|0,0,0) \)

(5) \( \overline{1} \)
    \( 0,0,0 \)
    \( (1|0,0,0)' \)

(6) \( m \)
    \( x,y,1/4 \)
    \( (m_z|0,0,1/2) \)

(7) \( c \)
    \( (0,0,1/2) \)
    \( x,0,z \)
    \( (m_y|0,0,1/2) \)

(8) \( m' \)
    \( 0,y,z \)
    \( (m'_z|0,0,0)' \)

For (1/2,1/2,0) + set

(1) \( t \)
    \( (1/2,1/2,2,0) \)
    \( (1|1/2,1/2,2,0) \)

(2) \( 2' \)
    \( (0,0,1/2) \)
    \( 1/4,1/4,z \)
    \( (2_z|1/2,1/2,1/2)' \)

(3) \( 2' \)
    \( (0,1/2,0) \)
    \( 1/4,y,1/4 \)
    \( (2_y|1/2,1/2,1/2)' \)

(4) \( 2 \)
    \( x,1/4,0 \)
    \( (2_x|1/2,1/2,0) \)

(5) \( \overline{1} \)
    \( 1/4,1/4,0 \)
    \( (1|1/2,1/2,0)' \)

(6) \( n \)
    \( (1/2,1/2,2,0) \)
    \( x,y,1/4 \)
    \( (m_z|1/2,1/2,1/2) \)

(7) \( n \)
    \( (1/2,0,1/2) \)
    \( x,1/4,z \)
    \( (m_y|1/2,1/2,1/2) \)

(8) \( b' \)
    \( (0,1/2,0) \)
    \( 1/4,y,z \)
    \( (m_z|1/2,1/2,0)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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<td>16 h</td>
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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>(3) x,y,z+1/2 [u,v,w]</td>
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<td>(7) x,y,z+1/2 [u,v,w]</td>
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<td>(8) x,y,z [u,v,w]</td>
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<td>x,y,1/4 [0,0,w]</td>
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<td>8 f m'</td>
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<td>8 e 2</td>
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<td>1/4,1/4,0 [0,0,0]</td>
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<td>4 c m'2m</td>
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<tr>
<td>4 b 2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
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<tr>
<td>4 a 2/m'</td>
<td>0,0,0 [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1] c2mm1'  Along [1,0,0] p2mg  Along [0,1,0] p2a' 2m'm'
a* = a  b* = b  a* = c  b* = b/2  a* = c/2  b* = a/2
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Orthorhombic

Cmc'\text{m}

63.4.514

mm'\text{m}

C2'/m2/c'2, '/m

Origin at (2'/m) at 2'/mc'2, '

Asymmetric unit

0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1 | 0,0,0)
(2) 2' \ (0,0,1/2) \ 0,0,z
   (2_z | 0,0,1/2)'
(3) 2 \ 0,y,1/4
   (2_y | 0,0,1/2)
(4) 2' \ x,0,0
   (2_x | 0,0,0)'

(5) \text{\overline{1}} \ 0,0,0
   (1 | 0,0,0)'
(6) m \ x,y,1/4
   (m_z | 0,0,1/2)
(7) c' \ (0,0,1/2) \ x,0,z
   (m_y | 0,0,1/2)'
(8) m \ 0,y,z
   (m_z | 0,0,0)

For (1/2,1/2,0) + set

(1) t \ (1/2,1/2,2,0)
   (1 | 1/2,1/2,2,0)
(2) 2' \ (0,0,1/2) \ 1/4,1/4,z
   (2_z | 1/2,1/2,1,2)'
(3) 2 \ (0,1/2,0) \ 1/4,y,1/4
   (2_y | 1/2,1,2,1/2)
(4) 2' \ (1/2,0,0) \ x,1/4,0
   (2_x | 1/2,1/2,0)'

(5) \text{\overline{1}} \ 1/4,1/4,0
   (1 | 1/2,1/2,2,0)'
(6) n \ (1/2,1/2,2,0) \ x,y,1/4
   (m_z | 1/2,1/2,1/2)
(7) n' \ (1/2,0,1/2) \ x,1/4,z
   (m_y | 1/2,1/2,1/2)'
(8) b \ (0,1/2,0) \ 1/4,y,z
   (m_z | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
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<td>(1) x,y,z [u,v,w]</td>
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<td>8 f m..</td>
<td>0,y,z [u,0,0]</td>
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<tr>
<td>8 e 2'..</td>
<td>x,0,0 [0,v,w]</td>
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<tr>
<td>8 d 1</td>
<td>1/4,1/4,0 [0,0,0]</td>
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<tr>
<td>4 c m2m</td>
<td>0,y,1/4 [0,0,0]</td>
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<tr>
<td>4 b 2'/m..</td>
<td>0,1/2,0 [0,0,0]</td>
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<td>4 a 2'/m..</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1'  
Along [1,0,0] p2mg1'  
Along [0,1,0] p2mm

\( a^* = a \) \( b^* = b \)  
\( a^* = -c \) \( b^* = b/2 \)  
\( a^* = c/2 \) \( b^* = a/2 \)

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at (2/m) at 2/mc$_2$.

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

1. 1
2. 2 (0,0,1/2) 0,0,z
3. 2' 0,y,1/4
4. 2' x,0,0
5. m' 0,0,0
6. m' x,y,1/4
7. c (0,0,1/2) x,0,z
8. m 0,y,z

For (1/2,1/2,0) + set

1. t (1/2,1/2,0)
2. 2 (0,0,1/2) 1/4,1/4,z
3. 2' (0,1/2,0) 1/4,y,1/4
4. 2' (1/2,0,0) x,1/4,0
5. n' 1/2,1/4,0
6. m' 1/2,1/2,1/2'
7. n 1/2,1/2,1/2'
8. b (0,1/2,0) 1/4,y,z
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>16 h</td>
<td>(0,0,0) +</td>
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<tr>
<td>16</td>
<td>(1/2,1/2,0) +</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
</tr>
<tr>
<td>b* = b</td>
</tr>
</tbody>
</table>

Along [1,0,0] p2mg1' a* = -c b* = b/2

Along [0,1,0] p2a, 2mm a* = c/2 b* = a/2

Origin at 0,0,0

Origin at x,0,0

Origin at 0,y,0
Origin at (2/m') at 2/m'c'2,

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)
(5) 1/2,1/2,0
(1 | 0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2z | 0,0,1/2)
(6) m x,y,1/4
(mz | 0,0,1/2)

(3) 2' 0,y,1/4
(2'y | 0,0,1/2)
(7) c' (0,0,1/2) x,0,z
(c | 0,0,1/2)

(4) 2' x,0,0
(2'y | 0,0,0)
(8) m' 0,y,z
(mz | 0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2z | 1/2,1/2,1/2)
(6) n (1/2,1/2,0) x,y,1/4
(mz | 1/2,1/2,1/2)

(3) 2' (0,1/2,0) 1/4,y,1/4
(2'y | 1/2,1/2,1/2)
(7) n' (1/2,0,1/2) x,1/4,z
(n | 1/2,1/2,1/2)

(4) 2' (1/2,0,0) x,1/4,0
(2'y | 1/2,1/2,0)
(8) b' (0,1/2,0) 1/4,y,z
(b | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

## Positions

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<tr>
<th>Multiplicity</th>
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</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td></td>
</tr>
<tr>
<td>(1/2,1/2,0) +</td>
<td></td>
</tr>
</tbody>
</table>

| 16 | h | 1 | (1) x,y,z [u,v,w] | (2) \(x, y, z + 1/2 [u, v, w]\) | (3) \(x, y, z + 1/2 [u, v, w]\) | (4) \(x, y, z [u, v, w]\) |
| 8  | g | .m | x,y,1/4 [0,0,w] | x,y,3/4 [0,0,w] | x,y,1/4 [0,0,w] | x,y,3/4 [0,0,w] |
| 8  | f | m'.. | 0,y,z [0,v,w] | 0,y,z+1/2 [0,v,w] | 0,y,z+1/2 [0,v,w] | 0,y,z [0,v,w] |
| 8  | e | 2'.. | x,0,0 [0,v,w] | x,0,1/2 [0,v,w] | x,0,0 [0,v,w] | x,0,1/2 [0,v,w] |
| 8  | d | 1 | 1/4,1/4,0 [u,v,w] | 3/4,3/4,1/2 [u,v,w] | 3/4,1/4,1/2 [u,v,w] | 1/4,3/4,0 [u,v,w] |
| 4  | c | m'2'm | 0,y,1/4 [0,0,w] | 0,y,3/4 [0,0,w] |
| 4  | b | 2'/m'.. | 0,1/2,0 [0,v,w] | 0,1/2,1/2 [0,v,w] |
| 4  | a | 2'/m'.. | 0,0,0 [0,v,w] | 0,0,1/2 [0,v,w] |

**Symmetry of Special Projections**

- Along [0,0,1]  c2mm1'
  - \(a^* = a\) \(b^* = b\)
  - Origin at 0,0,z
- Along [1,0,0]  p2'mg'
  - \(a^* = -c\) \(b^* = b/2\)
  - Origin at x,0,0
- Along [0,1,0]  p 2'mm'
  - \(a^* = c/2\) \(b^* = a/2\)
  - Origin at 0,y,0
**Cmc'm'**

63.7.517

**mm'm'**

C2/m2/c'2, 'm'

---

**Origin** at (2/m) at 2/mc'2,'

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

**Symmetry Operations**

For (0,0,0) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>2</td>
<td>2' (0,0,1/2)</td>
<td>0,0,z</td>
</tr>
<tr>
<td>3</td>
<td>2'</td>
<td>(0,0,1/2)'</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>x,0,0</td>
</tr>
<tr>
<td>5</td>
<td>0,0,0</td>
<td>(0,0,1/2)'</td>
</tr>
<tr>
<td>6</td>
<td>m'</td>
<td>x,y,1/4</td>
</tr>
<tr>
<td>7</td>
<td>c' (0,0,1/2)</td>
<td>x,0,z</td>
</tr>
<tr>
<td>8</td>
<td>m</td>
<td>0,y,z</td>
</tr>
</tbody>
</table>

For (1/2,1/2,0) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>t (1/2,1/2,0)</td>
<td>(1/2,1/2,0)</td>
</tr>
<tr>
<td>2</td>
<td>2' (0,0,1/2)</td>
<td>1/4,1/4,z</td>
</tr>
<tr>
<td>3</td>
<td>2' (0,1/2,0)</td>
<td>1/4,y,1/4</td>
</tr>
<tr>
<td>4</td>
<td>2 (1/2,0,0)</td>
<td>x,1/4,0</td>
</tr>
<tr>
<td>5</td>
<td>1/4,1/4,0</td>
<td>(1/2,1/2,0)'</td>
</tr>
<tr>
<td>6</td>
<td>n' (1/2,1/2,0)</td>
<td>x,1/4,z</td>
</tr>
<tr>
<td>7</td>
<td>n' (1/2,0,1/2)</td>
<td>x,1/4,z</td>
</tr>
<tr>
<td>8</td>
<td>b (0,1/2,0)</td>
<td>1/4,0,0</td>
</tr>
</tbody>
</table>

---

63.7.517 - 1 - 1024
Generators selected

\((1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5)\).

**Positions**

Multiplicities, Wyckoff letters, Site Symmetries.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 h</td>
<td>(x,y,z\ [u,v,w])</td>
</tr>
<tr>
<td>16 h</td>
<td>(x,y,z+1/2\ [u,v,w])</td>
</tr>
<tr>
<td>16 h</td>
<td>(x,y,z+1/2\ [u,v,w])</td>
</tr>
<tr>
<td>8 g</td>
<td>(x,y,1/4\ [u,v,0])</td>
</tr>
<tr>
<td>8 g</td>
<td>(x,y,3/4\ [u,v,0])</td>
</tr>
<tr>
<td>8 f</td>
<td>(0,y,z\ [u,0,0])</td>
</tr>
<tr>
<td>8 e</td>
<td>(x,0,0\ [u,0,0])</td>
</tr>
<tr>
<td>8 e</td>
<td>(x,0,1/2\ [u,0,0])</td>
</tr>
<tr>
<td>8 d</td>
<td>(1/4,1/4,0\ [u,v,w])</td>
</tr>
<tr>
<td>8 d</td>
<td>(3/4,3/4,1/2\ [u,v,w])</td>
</tr>
<tr>
<td>4 c</td>
<td>(0,y,1/4\ [u,0,0])</td>
</tr>
<tr>
<td>4 b</td>
<td>(0,1/2,0\ [u,0,0])</td>
</tr>
<tr>
<td>4 a</td>
<td>(0,0,0\ [u,0,0])</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along \([0,0,1]\) p 2 mm' \(a^* = a\) \(b^* = b\)

Along \([1,0,0]\) p 2 mg1' \(a^* = -c\) \(b^* = b/2\)

Along \([0,1,0]\) p 2 mm' \(a^* = -a/2\) \(b^* = c/2\)
Origin at ( 2'/m' ) at 2'/m'c2,;

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2' (0,0,1/2) 0,0,z
(2' | 0,0,1/2)

(3) 2 0,y,1/4
(2 | 0,0,1/2)

(4) 2' x,0,0
(2' | 0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)

(2) 2' (0,0,1/2) 1/4,1/4,z
(2' | 1/2,1/2,1/2)

(3) 2 (0,1/2,0) 1/4,y,1/4
(2 | 1/2,1/2,1/2)

(4) 2' (1/2,0,0) x,1/4,0
(2' | 1/2,1/2,0)

(5) t 1/4,1/4,0
(1 | 1/2,1/2,0)

(6) n' (1/2,1/2,0) x,y,1/4
(m | 1/2,1/2,1/2)

(7) n (1/2,0,1/2) x,1/4,z
(m | 1/2,1/2,1/2)

(8) b' (0,1/2,0) 1/4,y,z
(m | 1/2,1/2,0)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

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<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
</tbody>
</table>

**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

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**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm'</th>
<th>Along [1,0,0]</th>
<th>p2'm'g</th>
<th>Along [0,1,0]</th>
<th>p2a, 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a</td>
<td>a* = -c</td>
<td>b* = b/2</td>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,1/4</td>
<td></td>
</tr>
</tbody>
</table>

63.8.518 - 2 - 1027
Origin at (2/m') at 2/m'c',

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

1. 1
   (1 | 0,0,0)

2. (0,0,1/2) 0,0,z
   (2 | 0,0,1/2)

3. 2 0,y,1/4
   (2 | 0,0,1/2)

4. 2 x,0,0
   (2 | 0,0,0)

5. 1/m' 0,0,0
   (1 | 0,0,0)

6. m' x,y,1/4
   (m | 0,0,1/2)

7. c' (0,0,1/2) x,0,z
   (m | 0,0,1/2)

8. m' 0,y,z
   (m | 0,0,0)

For (1/2,1/2,0) + set

1. t (1/2,1/2,2,0)
   (1 | 1/2,1/2,2,0)

2. (0,0,1/2) 1/4,1/4,z
   (2 | 1/2,1/2,1/2)

3. 2 (0,1/2,0) 1/4,y,1/4
   (2 | 1/2,1/2,1/2)

4. 2 (1/2,0,0) x,1/4,0
   (2 | 1/2,1/2,0)

5. 1/m' 1/4,1/4,0
   (1 | 1/2,1/2,0)

6. n' (1/2,1/2,2,0) x,y,1/4
   (m | 1/2,1/2,1/2)

7. n' (1/2,0,1/2) x,1/4,z
   (m | 1/2,1/2,1/2)

8. b' (0,1/2,0) 1/4,y,z
   (m | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

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</tr>
<tr>
<td>16 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 g .m'</td>
<td>x,y,1/4 [u,v,0]</td>
</tr>
<tr>
<td>8 f m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 e 2..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>8 d 1'</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c m'2m'</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>4 b 2/m'..</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2/m'..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2m'm'  Along [1,0,0] p2m'g'  Along [0,1,0] p2m'm'
\(a^* = a\)  \(b^* = b\)  \(a^* = c/2\)  \(b^* = a/2\)
Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Orthorhombic

Cp mcm

63.10.520

mmm1'

Cp 2/m 2/c 2/m

Origin at (2/m) at 2/mc2,

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2|0,0,1/2)

(3) 2 0,y,1/4
(2|0,0,1/2)

(4) 2 x,0,0
(2|0,0,0)

(5) m 0,0,0
(m0,0,0)

(6) m x,y,1/4
(m0,0,0)

(7) m (0,0,1/2) x,0,z
(m0,0,1/2)

(8) m 0,y,z
(m0,0,0)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(1|0,0,0)

(2) t' (0,0,1/2)
(0,0,1/2)

(3) 2' (0,1/2,0) 1/4,y,1/4
(0,1/2,0)

(4) 2' (1,2,0,0) x,1/4,0
(1,2,0,0)

(5) t' 1/4,1/4,0
(1|0,0,0)

(6) t' (1/2,1/2,0) x,y,1/4
(1/2,1/2,0)

(7) t' (0,1/2,0) x,1/4,1/4
(0,1/2,0)

(8) t' (1,2,1/2,0) x,1/4,0
(1,2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
<td></td>
</tr>
<tr>
<td>16 h 1</td>
<td>(1) x,y,z [u,v,w] (2) x',y',z+1/2 [u',v',w'] (3) x,y,z+1/2 [u,v,w] (4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 g ..m</td>
<td>(5) x',y',z [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) x,y,z+1/2 [u,v,w] (8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f m..</td>
<td>x,y,1/4 [0,0,w] x',y,3/4 [0,0,w] x,y,1/4 [0,0,w] x,y,3/4 [0,0,w]</td>
</tr>
<tr>
<td>8 e 2..</td>
<td>0,y,z [u,0,0] 0,y,z+1/2 [u,0,0] 0,y,z+1/2 [u,0,0] 0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 d 1</td>
<td>x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 1/4,3/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c m2m</td>
<td>0,y,1/4 [0,0,0] 0,y,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2/m..</td>
<td>0,1/2,0 [u,0,0] 0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 a 2/m..</td>
<td>0,0,0 [u,0,0] 0,0,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1' a* = a  b* = b
Along [1,0,0] p2mg1' a* = -c  b* = b/2
Origin at 0,0,z Origin at x,0,0

Along [0,1,0] p2221 a* = c/2  b* = a/2
Origin at 0,y,1/4
Orthorhombic

C\textsubscript{p}m'cm

63.11.521

mmm1'

C\textsubscript{p}2/m'2'/c2'\textsubscript{1}/m

Origin at (2/m') at 2/m'c2'\textsubscript{1}

Asymmetric unit

0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z
(2_2|0,0,1/2)'

(3) 2' 0,y,1/4
(2_2|0,0,1/2)'

(4) 2 x,0,0
(2_x|0,0,0)

(5) m' 0,0,0
(1|0,0,0)'

(6) m x,y,1/4
(m_x|0,0,1/2)

(7) c (0,0,1/2) x,0,z
(m_y|0,0,1/2)

(8) m' 0,y,z
(m_z|0,0,0)'

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)'
(1|1/2,1/2,0)'

(2) 2 (0,0,1/2) 1/4,1/4,z
(2_2|1/2,1/2,1/2)

(3) 2 (0,1/2,0) 1/4,y,1/4
(2_2|1/2,1/2,1/2)

(4) 2' (1/2,0,0) x,1/4,0
(2_x|1/2,1/2,0)'

(5) n' (1/2,1/2,0) x,y,1/4
(m_z|1/2,1/2,1/2)'

(7) n' (1/2,0,1/2) x,1/4,z
(m_y|1/2,1/2,1/2)'

(8) b (0,1/2,0) 1/4,y,z
(m_z|1/2,1/2,0)
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 h</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 g</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 f</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 e</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 d</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 c</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 b</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 a</td>
<td>((0,0,0) + (1/2,1/2,0)) +</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] \( c2mm \)
  \( a^* = a \)
  \( b^* = b \)
  Origin at 0,0,z

- Along [1,0,0] \( p_{2b} \)
  \( a^* = -c \)
  \( b^* = b/2 \)
  Origin at x,0,0

- Along [0,1,0] \( p_{\infty} \)
  \( a^* = c/2 \)
  \( b^* = a/2 \)
  Origin at 1/4,y,1/4
Cp,m'cm

63.12.522

mmm1'

Cp2'/m2/c2', /m

Ortorhombic

Origin at (2'/m) at 2'/mc'2',

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1

(1|0,0,0)

(2) 2' (0,0,1/2) 0,0,z

(2|0,0,1/2')

(3) 2' 0,y,1/4

(2|0,0,1/2)

(4) 2' x,0,0

(2|0,0,0)

For (1/2,1/2,0) + set

(1) t' (1/2,1/2,0)

(1|1/2,1/2,0')

(2) 2 (0,0,1/2) 1/4,1/4,z

(2|1/2,1/2,1/2)

(3) 2' (0,1/2,0) 1/4,y,1/4

(2|1/2,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0

(2|1/2,1/2,0)

For (1/2,1/2,0) + set

(5) 1/4,1/4,0

(1|1/2,1/2,0')

(6) n' (1/2,1/2,0) x,y,1/4

(1/2,1/2,1/2')

(7) n (1/2,0,1/2) x,1/4,z

(1/2,1/2,1/2')

(8) b' (0,1/2,0) 1/4,y,z

(1/2,1/2,1/2)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0)′ +</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>h</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>g</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
</tr>
<tr>
<td>8</td>
<td>e</td>
</tr>
<tr>
<td>1</td>
<td>d</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]** c2mm 1′
  - $a^* = a$
  - $b^* = b$

- **Along [1,0,0]** p2mg 1′
  - $a^* = a$
  - $b^* = b/2$

- **Along [0,1,0]** $p_{2a} 2mm$
  - $a^* = c/2$
  - $b^* = a/2$

Origin at 0,0,z
Origin at x,0,0
Origin at 0,y,0
CPmcm’  Orthorhombic

63.13.523

mm1’  Orthorhombic

63.13.523  C2’/m2’/c21/m’

Origin at (2’/m) at 2’/mc21

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(5) T1 0,0,0
(1 | 0,0,0)’

(6) m’ x,y,1/4
(mz | 0,0,1/2)’

(7) c (0,0,1/2) x,0,z
(my | 0,0,1/2)

(8) m 0,y,z
(mz | 0,0,0)

For (1/2,1/2,0)’ + set

(1) t’ (1/2,1/2,0)
(1 | 1/2,1/2,0)’

(5) T1 1/4,1/4,0
(1 | 1/2,1/2,0)

(6) n (1/2,1/2,0) x,y,1/4
(mz | 1/2,1/2,1/2)

(7) n’ (1/2,0,1/2) x,1/4,z
(my | 1/2,1/2,1/2)’

(8) b’ (0,1/2,0) 1/4,y,z
(mz | 1/2,1/2,0)’

For (0,0,0) + set

(2) 2 (0,0,1/2) 0,0,z
(2z | 0,0,1/2)

(3) 2’ 0,y,1/4
(2z | 0,0,1/2)’

(4) 2’ x,0,0
(2z | 0,0,0)’

For (1/2,1/2,0)’ + set

(2) 2’ (0,0,1/2) 1/4,1/4,z
(2z | 1/2,1/2,1/2)’

(3) 2 (0,1/2,0) 1/4,y,1/4
(2y | 1/2,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2z | 1/2,1/2,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 h 1</td>
<td>(0,0,0) + (1/2,1/2,0') +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(2) x',y',z+1/2 [u',v',w]</td>
<td></td>
</tr>
<tr>
<td>(3) x',y',z+1/2 [u',v',w]</td>
<td></td>
</tr>
<tr>
<td>(4) x',y',z [u',v',w]</td>
<td></td>
</tr>
<tr>
<td>(5) x',y',z [u',v',w]</td>
<td></td>
</tr>
<tr>
<td>(6) x,y,z+1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(7) x,y,z+1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(8) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 g ..m'</td>
<td></td>
</tr>
<tr>
<td>x,y,1/4 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>x',y,3/4 [u',v',0]</td>
<td></td>
</tr>
<tr>
<td>x',y,1/4 [u',v',0]</td>
<td>x',y,3/4 [u',v',0]</td>
</tr>
<tr>
<td>8 f m..</td>
<td></td>
</tr>
<tr>
<td>0,y,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>0,y,z+1/2 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>0,y,z+1/2 [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 e 2'..</td>
<td></td>
</tr>
<tr>
<td>x,0,0 [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>x,0,1/2 [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>x,0,0 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>8 d 1</td>
<td></td>
</tr>
<tr>
<td>1/4,1/4,0 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>3/4,3/4,1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>3/4,1/4,1/2 [u,v,w]</td>
<td>1/4,3/4,0 [u,v,w]</td>
</tr>
<tr>
<td>4 c m2'm'</td>
<td></td>
</tr>
<tr>
<td>0,y,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>0,y,3/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b 2'/m..</td>
<td></td>
</tr>
<tr>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a 2'/m..</td>
<td></td>
</tr>
<tr>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm</th>
<th>Along [1,0,0]</th>
<th>p2mg1'</th>
<th>Along [0,1,0]</th>
<th>p..m 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a</td>
<td>b' = b</td>
<td>a' = -c</td>
<td>b' = b/2</td>
<td>a' = c/2</td>
<td>b' = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at (2'/m') at 2'/m'c'2,

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/4 \]

Symmetry Operations

For (0,0,0) + set

(1) \( \mathbb{T} (0,0,0) \)

(2) \( 2 (0,0,1/2) \) \( 0,0,z \)

(3) \( 2' (0,0,1/2) \)

(4) \( 2' x,0,0 \)

For (1/2,1/2,0)' + set

(1) \( t' (1/2,1/2,0) \)

(2) \( 2' (0,0,1/2) \) \( 1/4,1/4,z \)

(3) \( 2 (0,1/2,0) \) \( 1/4,y,1/4 \)

(4) \( 2 (1/2,0,0) \) \( x,1/4,0 \)

(5) \( \mathbb{T} 1/4,1/4,0 \)

(6) \( n (1/2,1/2,0) \) \( x,1/4 \)

(7) \( n (1/2,0,1/2) \) \( x,1/4,z \)

(8) \( b (0,1/2,0) \) \( 1/4,y,z \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0)(2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>16 h</td>
<td>1 x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>m x,y,1/4 [0,0,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>m' x,y,3/4 [0,0,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>2' x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>8 d</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>m'2 m 0,y,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>2'/m' 0,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td>4 a</td>
<td>2'/m' 0,0,0 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1'  
Along [1,0,0] p_{2b},2mg  
Along [0,1,0] p_{2a},2mm  

\( a^* = a \quad b^* = b \)  
\( a^* = -c \quad b^* = b/2 \)  
\( a^* = -a/2 \quad b^* = c/2 \)

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at 1/4,y,1/4
Origin at (2/m) at 2/mc'2,'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1 (1 | 0,0,0)
(2) 2' (0,0,1/2) 0,0,z
(3) 2' 0,y,1/4 (2 | 0,0,1/2)
(4) 2 x,0,0
(5) 1 & 0,0,0
(6) m' x,y,1/4 (m | 0,0,1/2)
(7) c' (0,0,1/2) x,0,z (m | 0,0,1/2)
(8) m 0,y,z (m | 0,0,0)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,2,0)
(2) 2 (0,0,1/2) 1/4,1/4,z (2 | 1/2,1/2,1/2)
(3) 2 (0,1/2,0) 1/4,y,1/4 (2 | 1/2,1/2,1/2)
(4) 2' (1/2,0,0) x,1/4,0 (2 | 1/2,1/2,0)
(5) t' 1/4,1/4,0 (1 | 2,1/2,0)
(6) n (1/2,1/2,0) x,y,1/4 (m | 1/2,1/2,1/2)
(7) n (1/2,0,1/2) x,1/4,z (m | 1/2,1/2,1/2)
(8) b' (0,1/2,0) 1/4,y,z (m | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicities,
Wyckoff letters,
Site symmetries.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 h</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>..m'</td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f m..</td>
<td>0,y,z [u,0,0]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>2..</td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 d</td>
<td>1/4,1/4,0</td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c m2m'</td>
<td>0,y,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b 2/m..</td>
<td>0,1/2,0 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a 2/m..</td>
<td>0,0,0 [u,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm' a\* = a  b\* = b
Along [1,0,0] p2mg1' a\* = -c  b\* = b/2
Along [0,1,0] p2a2m'm' a\* = a/2  b\* = c/2
Origin at 0,0,z  Origin at 0,0,z  Origin at 0,y,0
Orthorhombic

$\text{C}_{p}\text{m}'\text{cm}'$

$\text{mmm}1'$

$63.16.526$

$\text{C}_{p}2'/\text{m}'2/\text{c}2_1'/\text{m}'$

Origin at (2'/m'') at 2'/m'c2,

Asymmetric unit

$0 < x < 1/2; 0 < y < 1/2; 0 < z < 1/4$

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2' (0,0,1/2) 0,0,z
(2_ | 0,0,1/2)'

(3) 2 0,y,1/4
(2_ | 0,0,1/2)

(4) 2' x,0,0
(2_ | 0,0,0)

(5) 1/2,1/2,0)
(1 | 1/2,1/2,0)

(6) m' x,y,1/4
(m_ | 0,0,1/2)

(7) c (0,0,1/2) x,0,z
(m_ | 0,0,1/2)

(8) m' 0,y,z
(m_ | 0,0,0)

For (1/2,1/2,0)' + set

(1) 1/2,1/2,0)'
(1 | 1/2,1/2,0)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2_ | 1/2,1/2,1/2)

(3) 2' (0,1/2,0) 1/4,y,1/4
(2_ | 1/2,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2_ | 1/2,1/2,0)

(5) 1/2,1/2,0)'
(1 | 1/2,1/2,0)

(6) n (1/2,1/2,0) x,y,1/4
(m_ | 1/2,1/2,1/2)

(7) n' (1/2,0,1/2) x,1/4,z
(m_ | 1/2,1/2,1/2)

(8) b (0,1/2,0) 1/4,y,z
(m_ | 1/2,1/2,0)
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
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<tr>
<td>16 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>(3) x,y,z+1/2 [u,v,w]</td>
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<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td>(7) x,y,z+1/2 [u,v,w]</td>
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<td>(8) x,y,z [u,v,w]</td>
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<td>8 g ..m'</td>
<td>x,y,1/4 [u,v,0]</td>
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<td>x,y,3/4 [u,v,0]</td>
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<td>x,y,1/4 [u,v,0]</td>
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<td></td>
<td>x,y,3/4 [u,v,0]</td>
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<tr>
<td>8 f m'..'</td>
<td>0,y,z [0,v,w]</td>
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<tr>
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<td>0,y,z+1/2 [0,v,w]</td>
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<tr>
<td></td>
<td>0,y,z+1/2 [0,v,w]</td>
</tr>
<tr>
<td>8 e 2'..'</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [0,v,w]</td>
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<td>x,0,1/2 [0,v,w]</td>
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<tr>
<td>8 d 1'</td>
<td>1/4,1/4,0 [0,0,0]</td>
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<tr>
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<td>3/4,3/4,1/2 [0,0,0]</td>
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<td>1/4,3/4,0 [0,0,0]</td>
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<tr>
<td>4 c m'2m'</td>
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<td>0,y,3/4 [0,v,0]</td>
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<tr>
<td>4 b 2'/m'..'</td>
<td>0,1/2,0 [0,v,w]</td>
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<td>0,1/2,1/2 [0,v,w]</td>
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<tr>
<td>4 a 2'/m'...</td>
<td>0,0,0 [0,v,w]</td>
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<td>0,0,1/2 [0,v,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] c2mm'
Along [1,0,0] p_{ab2m}g'
Along [0,1,0] p_c2mm

a* = -b  b* = a
a* = -c  b* = b/2
a* = c/2  b* = a/2

Origin at 0,0,z  Origin at x,1/4,0  Origin at 1/4,y,0
Origin at \((2/m') at 2/m'c'2_1\)

Asymmetric unit \(0 \leq x \leq 1/2;\) \(0 \leq y \leq 1/2;\) \(0 \leq z \leq 1/4\)

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad (0,0,1/2) 0,0,z \\
(3) & \quad 2' 0,y,1/4 \\
(4) & \quad 2' x,0,0 \\
(5) & \quad 1' 0,0,0 \\
(6) & \quad m' x,y,1/4 \\
(7) & \quad c' (0,0,1/2) x,0,z \\
(8) & \quad m' 0,y,z \\
\end{align*}
\]

For \((1/2,1/2,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad t' (1/2,1/2,0) \\
(2) & \quad 2' (0,0,1/2) 1/4,1/4,z \\
(3) & \quad 2' (0,1/2,0) 1/4,y,1/4 \\
(4) & \quad 2' (1/2,0,0) x,1/4,0 \\
(5) & \quad 1/4,1/4,0 \\
(6) & \quad n (1/2,1/2,0) x,y,1/4 \\
(7) & \quad n (1/2,0,1/2) x,1/4,z \\
(8) & \quad b (0,1/2,0) 1/4,y,z \\
\end{align*}
\]
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
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<td></td>
</tr>
<tr>
<td>16h</td>
<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td>16(5)</td>
<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td>8</td>
<td>x,y,1/4 [u,v,0]</td>
<td>x,y,3/4 [u,v,0]</td>
</tr>
<tr>
<td>8</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z+1/2 [0,v,w]</td>
</tr>
<tr>
<td>8</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
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<tr>
<td>8</td>
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<td>3/4,3/4,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>0,y,1/4 [0,v,0]</td>
<td>0,y,3/4 [0,v,0]</td>
</tr>
<tr>
<td>4</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
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<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1] c2mm'     
Along [1,0,0] p2mg'     
Along [0,1,0] p2mm'  

\[ a^* = a \quad b^* = b \]  
\[ a^* = -c \quad b^* = b/2 \]  
\[ a^* = c/2 \quad b^* = a/2 \]  

Origin at 0,0,z          
Origin at x,0,0          
Origin at 0,y,0          

63.17.527 - 2 - 1045
Origin at center (2/m) at 2/mn1

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1 | 0,0,0)  
(5) 1/4,0,0
    (1) 0,0,0

(2) 2 (0,0,1/2) 0,1/4,z
    (2z | 0,1/2,1/2)
(6) b (0,1/2,0) x,y,1/4
    (mz | 0,1/2,1/2)
(7) c (0,0,1/2) x,1/4,z
    (my | 0,1/2,1/2)
(8) m 0,y,z
    (mx | 0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
    (1 | 1/2,1/2,0)
(5) 1/4,1/4,0
    (1 | 1/2,1/2,0)

(2) 2 (0,0,1/2) 1/4,0,z
    (2z | 1/2,0,1/2)
(6) a (1/2,0,0) x,y,1/4
    (mz | 1/2,0,1/2)
(7) n (1/2,0,1/2) x,0,z
    (my | 1/2,0,1/2)
(8) b (0,1/2,0) 1/4,y,z
    (mx | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 g</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) ( \bar{x}, \bar{y}, \bar{z} [u,v,w] )</td>
</tr>
<tr>
<td>8 f</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 e .2</td>
<td>1/4,y,1/4 [0,v,0]</td>
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<tr>
<td>8 d 2</td>
<td>x,0,0 [u,0,0]</td>
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<tr>
<td>8 c 1</td>
<td>1/4,1/4,0 [u,v,w]</td>
</tr>
<tr>
<td>4 b 2/m</td>
<td>1/2,0,0 [u,0,0]</td>
</tr>
<tr>
<td>4 a 2/m</td>
<td>0,0,0 [u,0,0]</td>
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</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1] p\( \bar{c} \)-2mm:
  - \( a^* = a/2 \) \( b^* = b/2 \)
  - Origin at 0,1/4,z

- **Along [1,0,0] p2mg1'**:
  - \( a^* = -c \) \( b^* = b/2 \)
  - Origin at x,0,0

- **Along [0,1,0] p_{2a}2mm**:
  - \( a^* = c/2 \) \( b^* = a/2 \)
  - Origin at 0,y,0
Cmca1'  mmm1'  Orthorhombic
64.2.529  

Origin at center (2/m1') at 2/mn11'

Symmetry Operations

For (0,0,0) + set

1. \( (1 \mid 0,0,0) \)
2. \( (2 \mid 0,0,1/2) \)  \( 0,1/4,z \)
3. \( (3 \mid 0,1/2,0) \)  \( 0,y,1/4 \)
4. \( (4 \mid x,0,0) \)

For (0,1/2,1/2,0) + set

1. \( (1 \mid 1/2,1/2,0) \)
2. \( (2 \mid 0,0,1/2) \)  \( 1/4,0,z \)
3. \( (3 \mid 1/4,y,1/4) \)
4. \( (4 \mid x,1/4,0) \)

For (0,0,0)' + set

1. \( (1 \mid 0,0,0)' \)
2. \( (2 \mid 0,0,1/2) \)  \( 0,1/4,z \)
3. \( (3 \mid 0,1/2,0) \)  \( 0,y,1/4 \)
4. \( (4 \mid x,0,0) \)

For (1/2,1/2,0)' + set

1. \( (1 \mid 1/2,1/2,0)' \)
2. \( (2 \mid 0,0,1/2) \)  \( 1/4,0,z \)
3. \( (3 \mid 1/4,y,1/4) \)
4. \( (4 \mid x,1/4,0) \)

Asymmetric unit

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5); 1'.

Positions

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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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<tbody>
<tr>
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<td>(0,0,0) + (0,0,0)’ +</td>
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<tr>
<td></td>
<td>(1/2,1/2,0) + (1/2,1/2,0)’ +</td>
</tr>
<tr>
<td>16 g 11' (1) x,y,z [0,0,0]</td>
<td>(2) (x, y + 1/2, z + 1/2) [0,0,0] (3) (x, y + 1/2, z + 1/2) [0,0,0]</td>
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<tr>
<td></td>
<td>(4) (x, y, z) [0,0,0]</td>
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<tr>
<td>(5) (\bar{x}, \bar{y}, \bar{z}) [0,0,0]</td>
<td>(6) (x, y + 1/2, z + 1/2) [0,0,0] (7) (x, y + 1/2, z + 1/2) [0,0,0]</td>
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<td>(8) (\bar{x}, \bar{y}, \bar{z}) [0,0,0]</td>
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<tr>
<td>8 f m..1' 0,y,z [0,0,0]</td>
<td>0,(y + 1/2, z + 1/2) [0,0,0] 0,(y + 1/2, z + 1/2) [0,0,0] 0,(y, z) [0,0,0]</td>
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<tr>
<td>8 e .2.1' 1/4,y,1/4 [0,0,0]</td>
<td>3/4,(y + 1/2, 3/4) [0,0,0] 3/4,(y, 3/4) [0,0,0] 1/4,(y + 1/2, 1/4) [0,0,0]</td>
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<tr>
<td>8 d 2..1' x,0,0 [0,0,0]</td>
<td>(\bar{x}, 1/2, 1/2) [0,0,0] (\bar{x}, 0, 0) [0,0,0] (x, 1/2, 1/2) [0,0,0]</td>
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<tr>
<td>8 c 11' 1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 1/4,3/4,0 [0,0,0]</td>
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<tr>
<td>4 b 2/m..1' 1/2,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>4 a 2/m..1' 0,0,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2mm1'</th>
<th>Along [1,0,0] p2mg1'</th>
<th>Along [0,1,0] p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a/2) (b^* = b/2)</td>
<td>(a^* = -c) (b^* = b/2)</td>
<td>(a^* = c/2) (b^* = a/2)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Cm'ca

64.3.530

m'mm

C2/m'2'/c2; '/a

Orthorhombic

**Origin** at center (2/m') at 2/m'n1

**Asymmetric unit**

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For (0,0,0) + set

1. \( \mathbf{1} \)  \( (0,0,0) \)
2. \( \mathbf{2'} \)  \( (0,0,1/2) \)  \( 0,1/4,z \)
3. \( \mathbf{2'} \)  \( (0,1/2,0) \)  \( 0,y,1/4 \)
4. \( \mathbf{2} \)  \( (0,0,0) \)

5. \( \mathbf{1'} \)  \( (0,0,0) \)
6. \( \mathbf{b} \)  \( (0,1/2,0) \)  \( x,y,1/4 \)
7. \( \mathbf{c} \)  \( (0,0,1/2) \)  \( x,1/4,z \)
8. \( \mathbf{m'} \)  \( (0,0,0) \)

For (1/2,1/2,0) + set

1. \( \mathbf{t} \)  \( (1/2,1/2,0) \)
2. \( \mathbf{2'} \)  \( (0,0,1/2) \)  \( 1/4,0,z \)
3. \( \mathbf{2'} \)  \( (1/2,0,0) \)  \( 1/4,y,1/4 \)
4. \( \mathbf{2} \)  \( (1/2,0,0) \)

5. \( \mathbf{1'} \)  \( (1/2,1/2,0) \)
6. \( \mathbf{a} \)  \( (1/2,0,0) \)  \( x,y,1/4 \)
7. \( \mathbf{n} \)  \( (1/2,0,1/2) \)  \( x,0,z \)
8. \( \mathbf{b'} \)  \( (0,1/2,0) \)  \( 1/4,y,z \)
Generators selected  \( t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5). \)

**Positions**

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</tr>
<tr>
<td>8</td>
<td>((1) x,y,z [u,v,w] )</td>
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<td></td>
<td>((2) \bar{x}, \bar{y}+1/2, \bar{z}+1/2 [u,v,w] )</td>
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<td>((3) \bar{x}, y+1/2, \bar{z}+1/2 [u,v,w] )</td>
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<td>((4) x,\bar{y},\bar{z} [u,v,w] )</td>
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<td>((5) \bar{x}, \bar{y}, \bar{z} [u,v,w] )</td>
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<td>((6) x,y+1/2, \bar{z}+1/2 [u,v,w] )</td>
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<td>((7) x,\bar{y}+1/2, \bar{z}+1/2 [u,v,w] )</td>
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<td>((8) \bar{x}, \bar{y}, \bar{z} [u,v,w] )</td>
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<td>8</td>
<td>(m'.. 0,y,z [0,v,w] )</td>
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<tr>
<td>8</td>
<td>(e ..2'. 1/4,y,1/4 [u,0,w] )</td>
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<tr>
<td>8</td>
<td>(d .. 2.. x,0,0 [u,0,0] )</td>
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<td>8</td>
<td>(c \bar{1}' 1/4,1/4,0 [0,0,0] )</td>
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<tr>
<td>4</td>
<td>(b 2/m'.. 1/2,0,0 [0,0,0] )</td>
</tr>
<tr>
<td>4</td>
<td>(a 2/m'.. 0,0,0 [0,0,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \ p2mm1'  \( b^* = b/2 \)
- Along \([1,0,0]\) \ p2mg  \( a^* = a/2 \)
- Along \([0,1,0]\) \ p_{2a'2m1'm'}  \( a^* = c/2 \)

Origin at \(0,0,z\)

Origin at \(x,0,0\)
Origin at center (2'/m) at 2'/mn'1

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)
(2') 2' (0,0,1/2) 0,1/4,z
(2 | 0,1/2,1/2)'
(3) 2 (0,1/2,0) 0,y,1/4
(2 | 0,1/2,1/2)
(4) 2' x,0,0
(2 | 0,0,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)
(2') 2' (0,0,1/2) 1/4,0,z
(2 | 1/2,0,1/2)'
(3) 2 1/4,y,1/4
(2 | 1/2,0,1/2)
(4) 2' (1/2,0,0) x,1/4,0
(2 | 1/2,1/2,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)
(2') 2' (0,0,1/2) 1/4,0,z
(2 | 1/2,0,1/2)'
(3) 2 1/4,y,1/4
(2 | 1/2,0,1/2)
(4) 2' (1/2,0,0) x,1/4,0
(2 | 1/2,1/2,0)'

(5) T' 1/4,1/4,0
(1 | 1/2,1/2,0)'
(6) a (1/2,0,0) x,y,1/4
(1 | 2,0,1/2)
(7) n' (1/2,0,1/2) x,0,z
(1 | 2,0,1/2)'
(8) b (0,1/2,0) 1/4,y,z
(1 | 2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 f</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 e</td>
<td>1/4,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 d</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>8 c</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p2-mm'</td>
<td>p2-mm'</td>
<td>p2mg1'</td>
<td>p2a-2mm</td>
</tr>
<tr>
<td>a* = a/2</td>
<td>a* = -c</td>
<td>a* = -a/2</td>
<td>a* = c/2</td>
</tr>
<tr>
<td>b* = b/2</td>
<td>b* = b/2</td>
<td>b* = b/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,1/4,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>


**Symmetry Operations**

For (0,0,0) + set

1. $t(1,0,0)$
2. $2 (0,0,1/2)$, $0,1/4,z$
3. $2' (0,1/2,0)$, $0,y,1/4$
4. $2' x,0,0$

For (1/2,1/2,0) + set

1. $t(1/2,1,2,0)$
2. $2 (0,0,1/2)$, $1/4,0,z$
3. $2' 1/4,y,1/4$
4. $2' (1/2,0,0)$, $x,1/4,0$

Origin at center (2/m) at 2/m1

Asymmetric unit: $0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>16 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
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<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y+1/2,z+1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y+1/2,z+1/2 [u,0,0]</td>
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<tr>
<td></td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 e .2'</td>
<td>1/4,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,y+1/2,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,y+1/2,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,y+1/2,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 d 2'..</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>8 c 1</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/4,3/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2'/m..</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2'/m..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2mm
  - a' = a/2
  - Origin at 0,0,z

- Along [1,0,0] p2mg1'
  - a' = -c
  - b' = b/2
  - Origin at x,0,0

- Along [0,1,0] p2a-2mm
  - a' = c/2
  - b' = a/2
  - Origin at 0,y,0
Origin at center (2'/m') at 2'/m'n'1

Asymmetric unit $0 < x < 1/4; \ 0 < y < 1/2; \ 0 < z < 1/2$

Symmetry Operations

For (0,0,0) + set

(1) $1$

$\begin{align*}
(1, 0, 0, 0) \\
(1, 1/2, 0, 0)
\end{align*}$

(2) $2 (0, 0, 1/2) \ 0, 1/4, z$

$\begin{align*}
(2, 0, 1/2, 0) \\
(2, 0, 1/2, 1/2)
\end{align*}$

(3) $2' (0, 1/2, 0) \ 0, y, 1/4$

$\begin{align*}
(2, 1/2, 0, 0) \\
(2, 1/2, 0, 1/2)
\end{align*}$

(4) $2' x, 0, 0$

$\begin{align*}
(2, 1/2, 0, 0) \\
(2, 1/2, 1/2, 0)
\end{align*}$$

\begin{align*}
(2, 0, 0, 0) \\
(2, 0, 0, 1/2)
\end{align*}$

(5) $0, 0, 0$

(6) $0, 1/2, 0)$

$\begin{align*}
(0, 1/2, 1/2) \\
(m, 0, 1/2, 1/2)
\end{align*}$

(7) $0, 1/2, 0) \ x, 1/4, z$

$\begin{align*}
(m, 1/2, 0, 0) \\
(m, 1/2, 0, 1/2)
\end{align*}$

(8) $0, y, z$

$\begin{align*}
(0, 1/2, 0) \\
(0, 1/2, 1/2)
\end{align*}$

For (1/2,1/2,1/2) + set

(1) $t (1/2, 1/2, 0)$

$\begin{align*}
(1, 1/2, 1/2, 0) \\
(1, 1/2, 2, 0)
\end{align*}$

(2) $2 (0, 0, 1/2) \ 1/4, 0, z$

$\begin{align*}
(2, 1/2, 0, 1/2) \\
(2, 1/2, 0, 1/2)
\end{align*}$

(3) $2' 1/4, y, 1/4$

$\begin{align*}
(2, 1/2, 2, 0, 0) \\
(2, 1/2, 2, 0, 1/2)
\end{align*}$

(4) $2' (1/2, 0, 0) \ x, 1/4, 0$

$\begin{align*}
(2, 1/2, 1/2, 0) \\
(2, 1/2, 1/2, 0)
\end{align*}$

(5) $1/4, 1/4, 0$

$\begin{align*}
(1/2, 1/4, 0) \\
(1/2, 1/4, 0)
\end{align*}$

(6) $a (1/2, 0, 0) \ x, y, 1/4$

$\begin{align*}
(m, 1/2, 0, 1/2) \\
(m, 1/2, 0, 1/2)
\end{align*}$

(7) $n' (1/2, 0, 1/2) \ x, 0, z$

$\begin{align*}
(m, 1/2, 0, 1/2) \\
(m, 1/2, 0, 1/2)
\end{align*}$

(8) $b' (0, 1/2, 0) \ 1/4, y, z$

$\begin{align*}
(m, 1/2, 0, 1/2) \\
(m, 1/2, 0, 1/2)
\end{align*}$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td>(0,0,0) +</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y+1/2,z+1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(8) x,y,z [u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

| 8 f          | 0,y,z [0,v,w] |               |
|              | 0,y+1/2,z+1/2 [0,v,w] |               |
| (1/2,0,0) [u,v,w] | (0,v,w) |               |

| 8 e          | 1/4,y,1/4 [u,0,w] |               |
|              | 3/4,y+1/2,3/4 [u,0,w] |               |
| 1/2,1/2,1/2 [u,0,w] | (0,v,w) |               |

| 8 d          | x,0,0 [0,v,w] |               |
|              | x,1/2,1/2 [0,v,w] |               |
| 1/2,1/2,1/2 [0,v,w] | (0,v,w) |               |

| 8 c          | 1/4,1/4,0 [u,v,w] |               |
|              | 3/4,1/4,1/2 [u,v,w] |               |
| 3/4,3/4,1/2 [u,v,w] | (0,v,w) |               |

| 4 b          | 1/2,0,0 [0,v,w] |               |
|              | 1/2,1/2,1/2 [0,v,w] |               |

| 4 a          | 0,0,0 [0,v,w] |               |
|              | 0,1/2,1/2 [0,v,w] |               |

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2/m'm'</th>
<th>Along [1,0,0] p2'mg'</th>
<th>Along [0,1,0] p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a/2</td>
<td>a* = -c</td>
<td>a* = c/2</td>
</tr>
<tr>
<td>b* = b/2</td>
<td>b* = b/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 1/4,y,1/4</td>
</tr>
</tbody>
</table>
Origin at center (2/m) at 2/mn'1

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) $1$
   
   (1) $0,0,0$

(2) $2' (0,1/2,0) \quad 0,1/4,z$
   
   (2) $0,1/2,1/2'$

(3) $2' (0,1/2,0) \quad 0,y,1/4$
   
   (3) $0,1/2,1/2'$

(4) $2 \quad x,0,0$
   
   (4) $2,0,0$

(5) $1$
   
   (5) $0,0,0$

(6) $b' (1/2,0,0) \quad x,y,1/4$
   
   (6) $1/2,0,1/2'$

(7) $c' (0,0,1/2) \quad x,1/4,z$
   
   (7) $0,1/2,1/2'$

(8) $m \quad 0,y,z$
   
   (8) $m,0,0,0$

For (1/2,1/2,0) + set

(1) $t (1/2,1/2,0)$
   
   (1) $1/2,1/2,0$

(2) $2' (0,1/2,0) \quad 1/4,0,z$
   
   (2) $1/2,0,1/2'$

(3) $2' \quad 1/4,y,1/4$
   
   (3) $1/2,0,1/2'$

(4) $2 \quad 1/2,0,0,0,0$
   
   (4) $2,1/2,1/2,0$

(5) $1$
   
   (5) $1/2,1/2,0$

(6) $a' (1/2,0,0) \quad x,y,1/4$
   
   (6) $1/2,0,1/2'$

(7) $n' (1/2,0,1/2) \quad x,0,z$
   
   (7) $1/2,0,1/2'$

(8) $b (0,1/2,0) \quad 1/4,y,z$
   
   (8) $1/2,1/2,0$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

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<td>(1) x,y,z [u,v,w]</td>
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<tr>
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<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
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<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
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<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<td>(6) x,y+1/2,z+1/2 [u,v,w]</td>
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<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
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<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>0,y,z [u,0,0]</td>
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<td>0,y+1/2,z+1/2 [u,0,0]</td>
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<tr>
<td>8 e</td>
<td>1/4,y,1/4 [u,0,w]</td>
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<td>3/4,y+1/2,3/4 [u,0,w]</td>
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<tr>
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<td>x,1/2,1/2 [u,0,0]</td>
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<td></td>
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<tr>
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</tr>
<tr>
<td>8 c</td>
<td>1/4,1/4,0 [u,v,w]</td>
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<td>3/4,1/4,1/2 [u,v,w]</td>
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<td>1/4,3/4,0 [u,v,w]</td>
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<tr>
<td>4 b</td>
<td>1/2,0,0 [u,0,0]</td>
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<tr>
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<td>1/2,1/2,1/2 [u,0,0]</td>
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<tr>
<td>4 a</td>
<td>0,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2' mm'</th>
<th>Along [1,0,0] p2mg 1'</th>
<th>Along [0,1,0] p2' mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a/2   b* = b/2</td>
<td>a* = c/2   b* = a/2</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Cm'ca'

64.8.535

m'm'2/c2, 'a'

Orthorhombic

Origin at center (2'/m') at 2'/m'n1

Asymmetric unit

0 < x < 1/4; 0 < y < 1/2; 0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 0,0,0)

(2) 2' (0,0,1/2) 0,1/4,z
(2z 0,1/2,1/2')

(3) 2 (0,1/2,0) 0,y,1/4
(2y 0,1/2,1/2)

(4) 2' x,0,0
(2x 0,0,0)

(5) 1/2,0,0
(1 0,0,0)

(6) b' (0,1/2,0) x,y,1/4
(mz 0,1/2,1/2')

(7) c (0,0,1/2) x,1/4,z
(my 0,1/2,1/2)

(8) m' 0,y,z
(mz 0,0,0')

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 1/2,1/2,0)

(2) 2' (0,0,1/2) 1/4,0,z
(2z 1/2,0,1/2')

(3) 2 1/4,y,1/4
(2y 1/2,0,1/2)

(4) 2' (1/2,0,0) x,1/4,0
(2x 1/2,1/2,0)

(5) 1/4,1/4,0
(1 1/2,1/2,0)

(6) a' (1/2,0,0) x,y,1/4
(mz 1/2,0,1/2')

(7) n (1/2,0,1/2) x,0,z
(my 1/2,0,1/2)

(8) b' (0,1/2,0) 1/4,y,z
(mz 1/2,1/2,0)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

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<td>(2) x,x+1/2,y+1/2 [u,v,w]</td>
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<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>1/4,y+1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 d</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>8 c</td>
<td>1/4,1/4 [0,v,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>1/2,0,0 [0,v,w]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2'2'm'

\[ a^* = -b/2 \quad b^* = a/2 \]

Origin at 0,0,z

Along [1,0,0] p2'm'g

\[ a^* = -c \quad b^* = b/2 \]

Origin at x,0,0

Along [0,1,0] p_{2a}2'm'

\[ a^* = c/2 \quad b^* = a/2 \]

Origin at 0,y,1/4
Cm'c'a'  
64.9.536  

m'm'm'  
C2/m'2/c'2,/a'

Orthonombic

Origin at center (2/m') at 2/m'n'1

Asymmetric unit  
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1 | 0,0,0)

(2) 2 (0,0,1/2) 0,1/4,z  
(2 | 0,1/2,1/2)

(3) 2 (0,1/2,0) 0,y,1/4  
(2 | 0,1/2,1/2)

(4) 2 x,0,0  
(2 | 0,0,0)

(5) T' 0,0,0  
(1 | 0,0,0)'

(6) b' (0,1/2,0) x,y,1/4  
(m, 0,1/2,1/2)'

(7) c' (0,0,1/2) x,1/4,z  
(m, 0,1/2,1/2)'

(8) m' 0,y,z  
(m, 0,0,0)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1 | 1/2,1/2,0)

(2) 2 (0,0,1/2) 1/4,0,z  
(2 | 1/2,0,1/2)

(3) 2 1/4,y,1/4  
(2 | 1/2,0,1/2)

(4) 2 (1/2,0,0) x,1/4,0  
(2 | 1/2,1/2,0)

(5) T' 1/4,1/4,0  
(1 | 2,1/2,0)'

(6) a' (1/2,0,0) x,y,1/4  
(m, 1/2,0,1/2)'

(7) n' (1/2,0,1/2) x,0,z  
(m, 1/2,0,1/2)'

(8) b' (0,1/2,0) 1/4,y,z  
(m, 1/2,1/2,0)'

64.9.536 - 1 - 1062
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

8 f  m'.. 0,y,z [0,v,w]  
8 e  .2. 1/4,y,1/4 [0,v,0]  
8 d  2.. x,0,0 [u,0,0]  
8 c  1/4,1/4,0 [0,0,0]  
4 b  2/m'. 1/2,0,0 [0,0,0]  
4 a  2/m'. 0,0,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p2m'm'  
Along [1,0,0] p2m'g'  
Along [0,1,0] p2m'm'

\[ a^* = a/2 \]  \[ b^* = b/2 \]  
\[ a^* = -c \]  \[ b^* = b/2 \]  
\[ a^* = c/2 \]  \[ b^* = a/2 \]  

Origin at 0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center (2/m) at 2/mn'1

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. 1
2. (0,0,1/2) 0,1/4,z
3. (0,1/2,0) 0,y,1/4
4. x,0,0
5. 0,0,0
6. (0,1/2,1/2) x,y,1/4
7. (0,0,1/2) x,1/4,z
8. 0,y,z

For (1/2,1/2,0)' + set

1. t' (1/2,1/2,0)
2. (0,0,1/2) 1/4,0,z
3. 1/4,y,1/4
4. (1/2,0,0) x,1/4,0
5. 1/2,1/2,0)
6. (0,1/2,0) x,y,1/4
7. (1/2,0,1/2) x,0,z
8. b' (0,1/2,0) 1/4,y,z

64.10.537 - 1 - 1064
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0):(2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x,y +1/2,z +1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) x,y +1/2,z +1/2 [u,v,w]</td>
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</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(6) x,y +1/2,z +1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) x,y +1/2,z +1/2 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

| 8 f m..      | 0,y,z [u,0,0]        |               |
| 8 e .2.      | 1/4,y,1/4 [0,v,0]    |               |
| 8 d 2..      | x,0,0 [u,0,0]        |               |
| 8 c 1'       | 1/4,1/4,0 [0,0,0]    |               |
| 4 b 2/m..    | 1/2,0,0 [u,0,0]      |               |
| 4 a 2/m..    | 0,0,0 [u,0,0]        |               |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2a-2mm</th>
<th>Along [1,0,0]</th>
<th>p2mg1'</th>
<th>Along [0,1,0]</th>
<th>p_c-2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -b/2</td>
<td>b* = a/2</td>
<td>a* = -c</td>
<td>b* = b/2</td>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,1/4,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 1/4,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Orthorhombic

$C_{p'm'ca}$

$64.11.538$

$mmm1'$

$C_{p2/m'2'/c21'/a}$

Origin at center (2/m') at 2/m'n'1

Asymmetric unit

$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

(1) $1$

(2) $2'$ (0,0,1/2) 0,1/4,z

(3) $2'$ (0,1/2,0) 0,y,1/4

(4) $2$ x,0,0

For (1/2,1/2,0)' + set

(5) $\bar{1}'$ 0,0,0

(6) $b$ (0,1/2,0) x,y,1/4

(7) $c$ (0,0,1/2) x,1/4,z

(8) $m'$ 0,y,z

For (1/2,1/2,0)' + set

(1) $t'$ (1/2,1/2,0)

(2) $2$ (0,0,1/2) 1/4,0,z

(3) $2$ 1/4,y,1/4

(4) $2'$ (1/2,0,0) x,1/4,0

(1/2,1/2,0)

(5) $\bar{1}$ 1/4,1/4,0

(6) $a'$ (1/2,0,0) x,y,1/4

(7) $n'$ (1/2,0,1/2) x,0,z

(8) $b$ (0,1/2,0) 1/4,y,z

(1/2,1/2,0)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + + (1/2,1/2,0)</td>
<td>(2) x, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u,v,w]</td>
<td></td>
<td>(3) x, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 f m'..</td>
<td>0,y,z [0,v,w]</td>
<td></td>
<td>(4) x, y, z [u,v,w]</td>
</tr>
<tr>
<td>8 e .2'</td>
<td>1/4, y, 1/4 [u,0,w]</td>
<td></td>
<td>(6) x, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 d 2..</td>
<td>x, 0, 0 [u,0,0]</td>
<td></td>
<td>(7) x, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 c 1</td>
<td>1/4, 1/4, 0 [u,v,w]</td>
<td></td>
<td>(8) x, y, z [u,v,w]</td>
</tr>
<tr>
<td>4 b 2/m'..</td>
<td>1/2, 0, 0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 a 2/m'..</td>
<td>0, 0, 0 [0,0,0]</td>
<td></td>
<td>0,1/2, 1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**  
  \( p_{2a}=2m'm' \)  
  \( a^* = -b/2 \quad b^* = a/2 \)  
  Origin at 0,0,z

- **Along [1,0,0]**  
  \( p2m'g' \)  
  \( a^* = -c \quad b^* = b/2 \)  
  Origin at x,0,0

- **Along [0,1,0]**  
  \( p_{c}=2mm \)  
  \( a^* = c/2 \quad b^* = a/2 \)  
  Origin at 1/4, y, 1/4
Origin at center (2’/m) at 2’/mn1

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1 | 0,0,0)
(2) 2’ (0,0,1/2) 0,1/4,z
    (2’ | 0,1/2,1/2)
(3) 2 (0,1/2,0) 0,y,1/4
    (2 | 0,1/2,1/2)
(4) 2’ x,0,0
    (2’ | 0,0,0)
(5) 1/4,1/4,0
    (1/4 | 0,0,0)
(6) b (0,1/2,0) x,y,1/4
    (m | 0,1/2,1/2)
(7) c’ (0,0,1/2) x,1/4,z
    (m’ | 0,1/2,1/2)
(8) m 0,y,z
    (m’ | 0,0,0)

For (1/2,1/2,0)’ + set

(1) t’ (1/2,1/2,0)
    (1/2 | 1/2,1/2,0)
(2) 2 (0,0,1/2) 1/4,0,z
    (2’ | 1/2,0,1/2)
(3) 2’ 1/4,y,1/4
    (2 | 1/2,0,1/2)
(4) 2 (1/2,0,0) x,1/4,0
    (2 | 1/2,1/2,0)
(5) 1/4,1/4,0
    (1/4 | 1/2,1/2,0)
(6) a’ (1/2,0,0) x,y,1/4
    (m | 1/2,0,1/2)
(7) n (1/2,0,1/2) x,0,z
    (m’ | 1/2,0,1/2)
(8) b’ (0,1/2,0) 1/4,y,z
    (m | 1/2,1/2,0)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td>16 g 1</td>
<td>(1) x,y,z [u,v,w] (2) x̃,ỹ+1/2,z+1/2 [ũ,ṽ,w̃] (3) x̃,ỹ+1/2,z+1/2 [ũ,ṽ,w̃] (4) x̃,ỹ,z [ũ,ṽ,w̃] (5) x̃,ỹ,z [ũ,ṽ,w̃] (6) x̃,ỹ+1/2,z+1/2 [ũ,ṽ,w̃] (7) x̃,ỹ+1/2,z+1/2 [ũ,ṽ,w̃] (8) x̃,ỹ,z [ũ,ṽ,w̃]</td>
</tr>
<tr>
<td>8 f m..</td>
<td>0,y,z [u,0,0] 0,ỹ+1/2,z+1/2 [ũ,0,0] 0,ỹ+1/2,z+1/2 [ũ,0,0] 0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 e .2.</td>
<td>1/4,y,1/4 [0,v,0] 3/4,y+1/2,3/4 [0,v,0] 3/4,ỹ+1/2,3/4 [0̃,ṽ,0] 1/4,y+1/2,1/4 [0̃,ṽ,0]</td>
</tr>
<tr>
<td>8 d 2'.</td>
<td>x,0,0 [0,v,w] x̃,1/2,1/2 [0̃,ṽ,w̃] x̃,0,0 [0̃,ṽ,w̃] x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>8 c 1</td>
<td>1/4,1/4,0 [u,v,w] 3/4,1/4,1/2 [ũ,ṽ,w̃] 3/4,3/4,1/2 [ũ,ṽ,w̃] 1/4,3/4,0 [u,v,w]</td>
</tr>
<tr>
<td>4 b 2'/m..</td>
<td>1/2,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2'/m..</td>
<td>0,0,0 [0,0,0] 0,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p_{2a}2mm, $a^* = -b/2$, $b^* = a/2$
- Along [1,0,0] p_{2mg}1', $a^* = -c$, $b^* = b/2$
- Along [0,1,0] p_{2a}2mm, $a^* = -a/2$, $b^* = c/2$
- Origin at 0,0,z
- Origin at x,0,0
- Origin at 0,y,0
Orthorhombic

Origin at center (2/m) at 2/mn'1

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For \((0,0,0)\) + set

1. \((1|0,0,0)\)  
2. \((2|0,0,1/2)\) \(0,1/4,z\)  
3. \((2'|0,1/2,0)\) \(0,y,1/4\)  
4. \((2'|0,0,0)\) \(x,0,0\)

5. \((\bar{1}|0,0,0)\)  
6. \((b'|0,1/2,0)\) \(x,y,1/4\)  
7. \((c|0,0,1/2)\) \(x,1/4,z\)  
8. \((a|0,1/2,0)\) \(1/4,y,z\)

For \((1/2,1/2,0)\) + set

1. \((t'|1/2,1/2,0)\)  
2. \((2'|0,0,1/2)\) \(1/4,0,z\)  
3. \((2|0,1/2,0)\) \(1/4,0,1/4\)  
4. \((2|1/2,0,0)\) \(1/4,0,0\)

5. \((\bar{1}|1/4,1/4,0)\)  
6. \((a|1/2,0,0)\) \(x,y,1/4\)  
7. \((n'|1/2,1/2,0)\) \(x,0,z\)  
8. \((b'|1/2,1/2,0)\) \(1/4,0,z\)

\[ 64.13.540 \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0)’ +</td>
</tr>
<tr>
<td>16 g</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>x,y+1/2,z+1/2 [u,v,w]</td>
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<td>x,y+1/2,z+1/2 [u,v,w]</td>
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<td></td>
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</tr>
<tr>
<td>8 f m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y+1/2,z+1/2 [u,0,0]</td>
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<tr>
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<td>0,y+1/2,z+1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 e .2'</td>
<td>1/4,y,1/4 [u,0,w]</td>
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<td>3/4,y+1/2,3/4 [u,0,w]</td>
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<td>3/4,y+1/2,3/4 [u,0,w]</td>
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<td>1/4,y+1/2,1/4 [u,0,w]</td>
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<tr>
<td>8 d 2'..</td>
<td>x,0,0 [0,v,w]</td>
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<td>x,1/2,1/2 [0,v,w]</td>
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<td>x,1/2,1/2 [0,v,w]</td>
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<td>8 c 1</td>
<td>1/4,1/4,0 [u,v,w]</td>
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<td>3/4,1/4,1/2 [u,v,w]</td>
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<td>1/4,3/4,0 [u,v,w]</td>
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<tr>
<td>4 b 2'/m..</td>
<td>1/2,0,0 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2a-2mm  

Along [1,0,0]  p2mg1'  

Along [0,1,0]  p_c-2mm  

\( a^* = a/2 \)  \( b^* = b/2 \)  

Origin at 0,0,z  

\( a^* = -c \)  \( b^* = b/2 \)  

Origin at x,0,0  

\( a^* = c/2 \)  \( b^* = a/2 \)  

Origin at 0,y,0
Origin at center (2'/m') at 2'/m'n1

Asymmetric unit
0 < x < 1/4;  0 < y < 1/2;  0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 (0,0,1/2) 0,1/4,z
(2z | 0,1/2,1/2)

(3) 2' (0,1/2,0) 0,y,1/4
(2z | 0,1/2,1/2)'

(4) 2' x,0,0
(2z | 0,0,0)'

(5) 1
(1 | 0,0,0)

(6) b (0,1/2,0) x,y,1/4
(mz | 0,1/2,1/2)

(7) c' (0,0,1/2) x,1/4,z
(my | 0,1/2,1/2)'

(8) m' 0,y,z
(mz | 0,0,0)'

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(1 | 1/2,1/2,0)'

(2) 2' (0,0,1/2) 1/4,0,z
(2z | 1/2,0,1/2)'

(3) 2 1/4,y,1/4
(2y | 1/2,0,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2z | 1/2,1/2,0)

(5) t' 1/4,1/4,0
(1 | 1/2,1/2,0)'

(6) a' (1/2,0,0) x,y,1/4
(mz | 1/2,0,1/2)'

(7) n (1/2,0,1/2) x,0,z
(my | 1/2,0,1/2)

(8) b (0,1/2,0) 1/4,y,z
(my | 1/2,1/2,0)
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0);(2); (3); (5)\).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td>((1) x,y,z [u,v,w] ) (2) (\bar{x},y+1/2,z+1/2 [u,v,w]) (3) (\bar{x},y+1/2,z+1/2 [u,v,w]) (4) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td>8 f</td>
<td>(m'.. ) (0,y,z [0,v,w] ) (0,y+1/2,z+1/2 [0,v,w] ) (0,y+1/2,z+1/2 [0,v,w] ) (0,y,z [0,v,w] )</td>
</tr>
<tr>
<td>8 e</td>
<td>(2'. ) (1/4,y,1/4 [u,0,w] ) (3/4,y+1/2,3/4 [u,0,w] ) (3/4,y,3/4 [u,0,w] ) (1/4,y+1/2,1/4 [u,0,w] )</td>
</tr>
<tr>
<td>8 d</td>
<td>(2'.. ) (x,0,0 [0,v,w] ) (\bar{x},1/2,1/2 [0,v,w] ) (\bar{x},0,0 [0,v,w] ) (x,1/2,1/2 [0,v,w] )</td>
</tr>
<tr>
<td>8 c</td>
<td>(\bar{1} ) (1/4,1/4,0 [0,0,0] ) (3/4,1/4,1/2 [0,0,0] ) (3/4,3/4,1/2 [0,0,0] ) (1/4,3/4,0 [0,0,0] )</td>
</tr>
<tr>
<td>4 b</td>
<td>(2'/m'.. ) (1/2,0,0 [0,v,w] ) (1/2,1/2,1/2 [0,v,w] )</td>
</tr>
<tr>
<td>4 a</td>
<td>(2'/m'.. ) (0,0,0 [0,v,w] ) (0,1/2,1/2 [0,v,w] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along ([0,0,1]) (p_{2a}2m'1m')</th>
<th>Along ([1,0,0]) (p_{2b}2mg)</th>
<th>Along ([0,1,0]) (p_{2a}2mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = -b/2) (b^* = a/2)</td>
<td>(a^* = -c) (b^* = b/2)</td>
<td>(a^* = -a/2) (b^* = c/2)</td>
</tr>
<tr>
<td>Origin at (0,1/4,z)</td>
<td>Origin at (x,1/4,0)</td>
<td>Origin at (1/4,y,1/4)</td>
</tr>
</tbody>
</table>
Origin at center (2/m) at 2/mn1

Asymmetric unit:

\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}\]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\, (0,0,0)\)
2. \(2'(0,0,1/2)\) \(0,1/4,z\)
3. \(2'(0,1/2,0)\) \(0,y,1/4\)
4. \(2 x,0,0\)

\(1^*\ (0,0,0)\)
\(2^* (0,1/2,1/2)\)
\(2^* (0,1/2,1/2)'\)
\(2^* (0,0,0)\)

5. \(1/4,0,0\)
\(0,1/2,1/2)\)
\(0,1/2,1/2)\)
\(0,1/2,1/2)\)

6. \(1/2,1/2,0\)
\(0,1/2,0)\) \(x,y,1/4\)
\(m_z,0,1/2,1/2)\)
\(m_z,0,1/2,1/2)\)

7. \(1/2,0,1/2)\)
\(0,1/2,0)\) \(x,1/4,z\)
\(m_y,0,1/2,1/2)\)
\(m_y,0,1/2,1/2)\)

8. \(m,0,y,z\)
\(m,0,y,z\)
\(m,0,y,z\)
\(m,0,y,z\)

For \((1/2,1/2,0)' + \) set

1. \(t' (1/2,1/2,0)\)
\(1/2,1/2,0)\)
\(1/2,1/2,0)\)
\(1/2,1/2,0)\)

2. \(2 (0,0,1/2)\) \(1/4,0,z\)
\(2 (1/2,0,1/2)\)
\(2 (1/2,0,1/2)\)
\(2 (1/2,0,1/2)\)

3. \(2 (1/2,0,1/2)\) \(1/4,y,1/4\)
\(2 (1/2,0,1/2)\)
\(2 (1/2,0,1/2)\)
\(2 (1/2,0,1/2)\)

4. \(2 (1/2,0,1/2)\) \(x,1/4,0\)
\(2 (1/2,0,1/2)\)
\(2 (1/2,0,1/2)\)
\(2 (1/2,0,1/2)\)

5. \(t^\prime (1/4,1/4,0)\)
\(1/2,1/2,0)\)
\(1/2,1/2,0)\)
\(1/2,1/2,0)\)

6. \(a (1/2,0,0)\) \(x,y,1/4\)
\(m_z,1/2,0,1/2)\)
\(m_z,1/2,0,1/2)\)
\(m_z,1/2,0,1/2)\)

7. \(n (1/2,0,1/2)\) \(x,0,z\)
\(m_y,1/2,0,1/2)\)
\(m_y,1/2,0,1/2)\)
\(m_y,1/2,0,1/2)\)

8. \(b' (0,1/2,0)\) \(1/4,y,z\)
\(m_z,1/2,1/2,0)'\)
\(m_z,1/2,1/2,0)'\)
\(m_z,1/2,1/2,0)'\)

64.15.542 - 1 - 1074
Generators selected \((1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5)\).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0)) +</td>
<td>((1/2,1/2,0)) +</td>
</tr>
<tr>
<td>16 g 1 ((1)) x,y,z [u,v,w]</td>
<td>((2)) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 f m.. 0,y,z [u,0,0]</td>
<td>0,y+1/2,z+1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 e .2'. 1/4,y,1/4 [u,0,w]</td>
<td>3/4,y+1/2,3/4 [u,0,w]</td>
</tr>
<tr>
<td>8 d 2.. x,0,0 [u,0,0]</td>
<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 c 1' 1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2/m.. 1/2,0,0 [u,0,0]</td>
<td>1/2,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 a 2/m.. 0,0,0 [u,0,0]</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along \([0,0,1]\) \(p_{2a}2m1m'\)
  - \(a^* = a/2\) \(b^* = b/2\)
  - Origin at 1/4,1/4,z

- **Along \([1,0,0]\) \(p2mg1'\)
  - \(a^* = c\) \(b^* = b/2\)
  - Origin at x,0,0

- **Along \([0,1,0]\) \(p_{2a}2m1m'\)
  - \(a^* = -a/2\) \(b^* = c/2\)
  - Origin at 0,y,0
**Origin** at center (2'/m') at 2'/m'n'

**Asymmetric unit**

\[ 0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \]

**Symmetry Operations**

For \((0,0,0) + \text{set}\):

1. \(1 \quad 0,0,0\)
2. \(2' \quad (0,0,1/2) \quad 0,1/4,z\)
3. \(2 \quad (0,1/2,0) \quad 0,y,1/4\)
4. \(2' \quad x,0,0\)

For \((1/2,1/2,0)' + \text{set}\):

1. \(t' \quad (1/2,1/2,0)\)
2. \(2 \quad (0,0,1/2) \quad 1/4,0,z\)
3. \(2' \quad 1/4,y,1/4\)
4. \(2 \quad (1/2,0,0) \quad x,1/4,0\)

\[ (\tau | 0,0,0) \]

1. \(b' \quad (0,1/2,0) \quad x,y,1/4\)
2. \(c \quad (0,0,1/2) \quad x,1/4,z\)
3. \(m' \quad 0,y,z\)
4. \(a \quad (1/2,0,0) \quad x,y,1/4\)
5. \(n' \quad (1/2,0,1/2) \quad x,0,z\)
6. \(b \quad (0,1/2,0) \quad 1/4,y,z\)

\[ (\tau | 1/2,1/2,0) \]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>16 g 1</td>
<td>(0,0,0) + (1/2,1/2,0)* +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(8) x,y,z [u,v,w]</td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f m..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 e .2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 d 2'..</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>8 c 1'</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2'/m'..</td>
<td>1/2,0,0 [0,v,w]</td>
</tr>
<tr>
<td>4 a 2'/m'..</td>
<td>0,0,0 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \(p_{2a}2mm\) \(a^* = a/2\ \ b^* = b/2\) Origin at 1/4,0,z
Along [1,0,0] \(p_{2b}2mg\) \(a^* = -c\ \ b^* = b/2\) Origin at x,1/4,0
Along [0,1,0] \(p_{c}2mm\) \(a^* = c/2\ \ b^* = a/2\) Origin at 1/4,y,0
Orthorhombic

64.17.544

$\text{C}_p m' c' a'$

$\text{mmm}_1' \quad \text{C}_p 2/m' 2/c' 2/a'$

**Origin** at center (2/m') at 2/m'n1

**Asymmetric unit** $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For (0,0,0) + set

1. $I$ (1|0,0,0)
2. $2 \cdot (0,0,1/2) \quad 0,1/4,z$
   (2$_z|0,1/2,1/2$)
3. $2 \cdot (0,1/2,0) \quad 0,y,1/4$
   (2$_y|0,1/2,1/2$)
4. $2 \cdot x,0,0$
   (2$_x|0,0,0$)

5. $T'$ 0,0,0
   (1|0,0,0)'
6. $b' \cdot (0,1/2,0) \quad x,y,1/4$
   (m$_z|0,1/2,1/2$)'
7. $c' \cdot (0,0,1/2) \quad x,1/4,z$
   (m$_y|0,1/2,1/2$)'
8. $m' \cdot 0,y,z$
   (m$_z|0,0,0$)'

For (1/2,1/2,0) + set

1. $t' \cdot (1/2,1/2,0)$
   (1|1/2,1/2,0)'
2. $2' \cdot (0,0,1/2) \quad 1/4,0,z$
   (2$_z|1/2,0,1/2$)'
3. $2' \cdot 1/4,y,1/4$
   (2$_y|1/2,0,1/2$)'
4. $2' \cdot (1/2,0,0) \quad x,1/4,0$
   (2$_x|1/2,1/2,0$)'

5. $T \cdot 1/4,1/4,0$
   (1|1/2,1/2,0)'
6. $a \cdot (1/2,0,0) \quad x,y,1/4$
   (m$_z|1/2,0,1/2$)
7. $n \cdot (1/2,0,1/2) \quad x,0,z$
   (m$_y|1/2,0,1/2$)
8. $b \cdot (0,1/2,0) \quad 1/4,y,z$
   (m$_z|1/2,1/2,0$)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>16 g 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 e .2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 d 2..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>8 c 1</td>
<td>1/4,1/4,0 [u,v,w]</td>
</tr>
<tr>
<td>4 b 2/m'..</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2/m'..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a•2m1'm'  
Along [1,0,0] p2b•2mg  
Along [0,1,0] p2a•2m1'm'  

\[ a^* = a/2 \quad b^* = b/2 \]  
\[ a^* = -c \quad b^* = b/2 \]  
\[ a^* = -a/2 \quad b^* = c/2 \]  

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Cmmm

65.1.545

Origin at center (mmm)

Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1|0,0,0)

(2) 2   0,0,z
    (2z|0,0,0)

(3) 2   0,y,0
    (2y|0,0,0)

(4) 2   x,0,0
    (2x|0,0,0)

(5) 1
    (1|0,0,0)

(6) m   x,y,0
    (mz|0,0,0)

(7) m   x,0,z
    (my|0,0,0)

(8) m   0,y,z
    (my|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
    (1|1/2,1/2,0)

(2) 2   1/4,1/4,z
    (2z|1/2,1/2,0)

(3) 2   (0,1/2,0)  1/4,y,0
    (2y|1/2,1/2,0)

(4) 2   (1/2,0,0)  x,1/4,0
    (2x|1/2,1/2,0)

(5) 1
    (1|1/2,1/2,0)

(2) 2   1/4,1/4,z
    (2z|1/2,1/2,0)

(3) 2   (0,1/2,0)  1/4,y,0
    (2y|1/2,1/2,0)

(4) 2   (1/2,0,0)  x,1/4,0
    (2x|1/2,1/2,0)

(5) 1
    (1|1/2,1/2,0)

(6) n (1/2,1/2,0)  x,y,0
    (mz|1/2,1/2,0)

(7) a (1/2,0,0)  x,1/4,z
    (my|1/2,1/2,0)

(8) b (0,1/2,0)  1/4,y,z
    (mz|1/2,1/2,0)
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).\)

**Positions**

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<tr>
<td>16 r 1</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 q ..m</td>
<td>(2) (x, y, z [u, v, w]) (3) (x, y, z [u, v, w]) (4) (x, y, z [u, v, w])</td>
</tr>
<tr>
<td>8 p ..m</td>
<td>(5) (x, y, z [u, v, w]) (6) (x, y, z [u, v, w]) (7) (x, y, z [u, v, w]) (8) (x, y, z [u, v, w])</td>
</tr>
<tr>
<td>8 o ..m</td>
<td>1/4,1/4,(z [0,0,w]) 3/4,1/4,(z [0,0,w]) 3/4,3/4,(z [0,0,w]) 1/4,3/4,(z [0,0,w])</td>
</tr>
<tr>
<td>4 l mm2</td>
<td>0,1/2,(z [0,0,0]) 0,1/2,(z [0,0,0])</td>
</tr>
<tr>
<td>4 k mm2</td>
<td>0,0,(z [0,0,0]) 0,0,(z [0,0,0])</td>
</tr>
<tr>
<td>4 j m2m</td>
<td>0,(y, 1/2 [0,0,0]) 0,(y, 1/2 [0,0,0])</td>
</tr>
<tr>
<td>4 i m2m</td>
<td>0,(y, 0 [0,0,0]) 0,(y, 0 [0,0,0])</td>
</tr>
<tr>
<td>4 h 2mm</td>
<td>(x, 0, 1/2 [0,0,0]) (x, 0, 1/2 [0,0,0])</td>
</tr>
<tr>
<td>4 g 2mm</td>
<td>(x, 0, 0 [0,0,0]) (x, 0, 0 [0,0,0])</td>
</tr>
<tr>
<td>4 f ..2/m</td>
<td>1/4,1/4,1/2 [0,0,w] 3/4,1/4,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 e ..2/m</td>
<td>1/4,1/4,0 [0,0,w] 3/4,1/4,0 [0,0,w]</td>
</tr>
<tr>
<td>2 d mmm</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c mmm</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b mmm</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a mmm</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) c2mm1'\(\quad\star a = a\quad b^* = b\star\)
- Along \([1,0,0]\) p2mm1'\(\quad a^* = b/2\quad b^* = c\star\)
- Along \([0,1,0]\) p2mm1'\(\quad a^* = c\quad b^* = a/2\star\)

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Orthorhombic

$$\text{Cmmm1'}$$

65.2.546

$$\text{mmm1'}$$

$$\text{C2/m2/m2/m1'}$$

Origin at center (mmm1')

Asymmetric unit

$$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$$

Symmetry Operations

For (0,0,0) + set

1. $$1$$  
   $$1'$$
2. $$2$$  $$0,0,z$$  
   $$0,0,0$$
3. $$2$$  $$0,y,0$$  
   $$0,0,0$$
4. $$2$$  $$0,0,0$$  
   $$0,0,0$$

For (1/2,1/2,0) + set

5. $$1'$$  $$1/2,1/2,0$$  
   $$1/2,1/2,0$$
6. $$2$$  $$1/4,1/4,z$$  
   $$1/2,1/2,2/0$$
7. $$2$$  $$0,1/2,0$$  
   $$1/2,1/2,2/0$$
8. $$2$$  $$0,1/2,0$$  
   $$1/2,1/2,2/0$$

For (0,0,0)' + set

9. $$1'$$  $$0,0,0$$  
   $$0,0,0$$
10. $$2'$$  $$0,0,z$$  
   $$0,0,0$$
11. $$2'$$  $$0,y,0$$  
   $$0,0,0$$
12. $$2'$$  $$0,0,0$$  
   $$0,0,0$$

For (1/2,1/2,0)' + set

13. $$1'$$  $$1/2,1/2,0$$  
   $$1/2,1/2,0$$
14. $$2'$$  $$1/4,1/4,z$$  
   $$1/2,1/2,2/0$$
15. $$2'$$  $$0,1/2,0$$  
   $$1/2,1/2,2/0$$
16. $$2'$$  $$0,1/2,0$$  
   $$1/2,1/2,2/0$$
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) + (0,0,0)’ +</td>
</tr>
<tr>
<td>16 r 11’ (1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0) + (1/2,1/2,0)’ +</td>
</tr>
<tr>
<td>8 q ..m1’ x,y,1/2 [0,0,0] x,y,1/2 [0,0,0] x,y,1/2 [0,0,0] x,y,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 p ..m1’ x,y,0 [0,0,0] x,y,0 [0,0,0] x,y,0 [0,0,0] x,y,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 o ..m1’ x,0,z [0,0,0] x,0,z [0,0,0] x,0,z [0,0,0] x,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
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<td></td>
</tr>
<tr>
<td>8 m ..21’ 1/4,1/4,z [0,0,0] 3/4,1/4,z [0,0,0] 3/4,3/4,z [0,0,0] 1/4,3/4,z [0,0,0]</td>
<td></td>
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<tr>
<td>4 l mm21’ 0,1/2,z [0,0,0] 0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 k mm21’ 0,0,z [0,0,0] 0,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 j m2m1’ 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 i m2m1’ 0,y,0 [0,0,0] 0,y,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 h 2mm1’ x,0,1/2 [0,0,0] x,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 g 2mm1’ x,0,0 [0,0,0] x,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 f ..2/m1’ 1/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e ..2/m1’ 1/4,1/4,0 [0,0,0] 3/4,1/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 d mmm1’ 0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 c mmm1’ 1/2,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b mmm1’ 1/2,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a mmm1’ 0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1’
a* = a  b* = b
Origin at 0,0,z
Along [1,0,0] p2mm1’
a* = b/2  b* = c
Origin at x,0,0
Along [0,1,0] p2mm1’
a* = c  b* = a/2
Origin at 0,y,0
### Origin
at center (m’mm)

### Asymmetric unit
0 \leq x < 1/4; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/2

### Symmetry Operations

**For (0,0,0) + set**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) (1)</td>
<td>(1</td>
</tr>
<tr>
<td>(2) (2')</td>
<td>(0,0,z) (2_z</td>
</tr>
<tr>
<td>(3) (2')</td>
<td>(0,y,0) (2_y</td>
</tr>
<tr>
<td>(4) (2)</td>
<td>((x,0,0)) (2_x</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5) (\overline{1})</td>
<td>(0,0,0) (\overline{1}</td>
</tr>
<tr>
<td>(6) (m)</td>
<td>(x,y,0) (m_x</td>
</tr>
<tr>
<td>(7) (m)</td>
<td>(x,0,z) (m_y</td>
</tr>
<tr>
<td>(8) (m')</td>
<td>(y,z) (m_z</td>
</tr>
</tbody>
</table>

**For (1/2,1/2,0) + set**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) (t)</td>
<td>((1/2,1/2,0)) ((1</td>
</tr>
<tr>
<td>(2) (2')</td>
<td>((1/4,1/4,z)) ((2_z</td>
</tr>
<tr>
<td>(3) (2')</td>
<td>((0,1/2,0)) ((2_y</td>
</tr>
<tr>
<td>(4) (2)</td>
<td>((x,1/4,0)) ((2_x</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5) (\overline{1})</td>
<td>((1/4,1/4,0)) ((\overline{1}</td>
</tr>
<tr>
<td>(6) (n)</td>
<td>((1/2,1/2,0)) ((m_z</td>
</tr>
<tr>
<td>(7) (a)</td>
<td>((1/2,0,0)) ((m_y</td>
</tr>
<tr>
<td>(8) (b')</td>
<td>((0,1/2,0)) ((m_z</td>
</tr>
</tbody>
</table>
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
<td>(0,0,0) +</td>
<td></td>
</tr>
<tr>
<td>16 r</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 q ..m</td>
<td>x,y,1/2 [0,0,0]</td>
<td>x,y,1/2 [0,0,0]</td>
<td>x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 p ..m</td>
<td>x,y,0 [0,0,0]</td>
<td>x,y,0 [0,0,0]</td>
<td>x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>8 o ..m</td>
<td>x,0,z [0,0,0]</td>
<td>x,0,z [0,0,0]</td>
<td>x,0,z [0,0,0]</td>
</tr>
<tr>
<td>8 n m' ..</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
</tr>
<tr>
<td>8 m ..2'</td>
<td>1/4,1/4,z [0,0,0]</td>
<td>3/4,1/4,z [0,0,0]</td>
<td>3/4,3/4,z [0,0,0]</td>
</tr>
<tr>
<td>4 l m'm2'</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 k m'm2'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 j m'2'm</td>
<td>0,y,1/2 [0,0,0]</td>
<td>0,y,1/2 [0,0,0]</td>
<td>0,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 i m'2'm</td>
<td>0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4 h 2mm</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 g 2mm</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 f ..2'/m</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e ..2'/m</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d m'mm</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c m'mm</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b m'mm</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a m'mm</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1'  
\[ a^* = a, b^* = b \]  
Origin at 0,0,0

Along [1,0,0] p2mm  
\[ a^* = b/2, b^* = c \]  
Origin at 0,0,0

Along [0,1,0] p2mm1'  
\[ a^* = c, b^* = a/2 \]  
Origin at 0,y,0
Origin at center (mmm')

Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. 1 0,0,0
2. 2 0,0,z
   (2z 0,0,0)
3. 2' 0,y,0
   (2z 0,0,0)'
4. 2' x,0,0
   (2z 0,0,0)'
5. m' 0,0,0
   (mz 0,0,0)'
6. m' x,y,0
   (mz 0,0,0)'
7. m x,0,z
   (mz 0,0,0)
8. m 0,y,z
   (mz 0,0,0)

For (1/2,1/2,0) + set

1. t (1/2,1/2,2,0)
   (1 1/2,1/2,2,0)
2. 2 1/4,1/4,z
   (2z 1/2,1/2,2,0)
3. 2' (0,1/2,0) 1/4,y,0
   (2z 1/2,1/2,2,0)'
4. 2' (1/2,0,0) x,1/4,0
   (2z 1/2,1/2,2,0)'
5. n' (1/2,1/2,2,0)
   (mz 1/2,1/2,2,0)'
6. n' x,y,0
   (mz 1/2,1/2,2,0)'
7. a (1/2,0,0) x,1/4,z
   (mz 1/2,1/2,2,0)
8. b (0,1/2,0) 1/4,y,z
   (mz 1/2,1/2,2,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 r 1</td>
<td>(1) x, y, z [u, v, w]</td>
<td>(0,0,0) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 q ..m'</td>
<td>x, y, 1/2 [u, v, 0]</td>
<td>x, y, 1/2 [u, v, 0]</td>
</tr>
<tr>
<td>8 p ..m'</td>
<td>x, y, 0 [u, v, 0]</td>
<td>x, y, 1/2 [u, v, 0]</td>
</tr>
<tr>
<td>8 o .m.</td>
<td>x, 0, z [0, v, 0]</td>
<td>x, 1/2 [u, v, 0]</td>
</tr>
<tr>
<td>8 n m..</td>
<td>0, y, z [u, 0, 0]</td>
<td>0, y, 1/2 [u, v, 0]</td>
</tr>
<tr>
<td>8 m ..2</td>
<td>1/4, 1/4, z [0, 0, w]</td>
<td>3/4, 3/4, z [0, 0, w]</td>
</tr>
<tr>
<td>4 l mm2</td>
<td>0, 1/2, z [0, 0, 0]</td>
<td>0, 1/2, z [0, 0, 0]</td>
</tr>
<tr>
<td>4 k mm2</td>
<td>0, 0, z [0, 0, 0]</td>
<td>0, 0, z [0, 0, 0]</td>
</tr>
<tr>
<td>4 j m2m'</td>
<td>0, y, 1/2 [u, 0, 0]</td>
<td>0, y, 1/2 [u, 0, 0]</td>
</tr>
<tr>
<td>4 i m2m'</td>
<td>0, y, 0 [u, 0, 0]</td>
<td>0, y, 0 [u, 0, 0]</td>
</tr>
<tr>
<td>4 h 2'mm'</td>
<td>x, 0, 1/2 [0, v, 0]</td>
<td>x, 0, 1/2 [0, v, 0]</td>
</tr>
<tr>
<td>4 g 2'mm'</td>
<td>x, 0, 0 [0, v, 0]</td>
<td>x, 0, 0 [0, v, 0]</td>
</tr>
<tr>
<td>4 f ..2/m'</td>
<td>1/4, 1/4, 1/2 [0, 0, 0]</td>
<td>3/4, 1/4, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>4 e ..2/m'</td>
<td>1/4, 1/4, 0 [0, 0, 0]</td>
<td>3/4, 1/4, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>2 d mmm'</td>
<td>0, 0, 1/2 [0, 0, 0]</td>
<td>0, 0, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>2 c mmm'</td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>2 b mmm'</td>
<td>1/2, 0, 0 [0, 0, 0]</td>
<td>1/2, 0, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>2 a mmm'</td>
<td>0, 0, 0 [0, 0, 0]</td>
<td>0, 0, 0 [0, 0, 0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Axes</th>
<th>Along [0, 0, 1]</th>
<th>c2mm</th>
<th>Along [1, 0, 0]</th>
<th>p2mm1'</th>
<th>Along [0, 1, 0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a*</td>
<td>= a</td>
<td></td>
<td>a* = b/2</td>
<td></td>
<td>a* = c</td>
<td></td>
</tr>
<tr>
<td>b*</td>
<td>= b</td>
<td></td>
<td>b* = c</td>
<td></td>
<td>b* = a/2</td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0, z  
Origin at x,0,0  
Origin at 0, y, 0

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Origin at center (m'm'm)

Asymmetric unit: $0 \leq x \leq 1/4$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

1. \( I \) (0,0,0)
2. \( 2 \) 0,0,z
   \( (2z \ 0,0,0) \)
3. \( 2' \) 0,y,0
   \( (2y \ 0,0,0)' \)
4. \( 2' \) x,0,0
   \( (2x \ 0,0,0)' \)
5. \( \bar{1} \) 0,0,0
   \( (1 \ 0,0,0) \)
6. \( m \) x,y,0
   \( (mz \ 0,0,0) \)
7. \( m' \) x,0,z
   \( (m'y \ 0,0,0)' \)
8. \( m' \) 0,y,z
   \( (m'z \ 0,0,0)' \)

For (1/2,1/2,0) + set

1. \( t \) (1/2,1/2,0)
   \( (1 \ 1/2,1/2,0) \)
2. \( 2 \) 1/4,1/4,z
   \( (2z \ 1/2,1/2,0) \)
3. \( 2' \) (0,1/2,0)
   \( 1/4,y,0 \)
   \( (2y \ 1/2,1/2,0)' \)
4. \( 2' \) (1/2,0,0)
   \( x,1/4,0 \)
   \( (2x \ 1/2,1/2,0)' \)
5. \( \bar{1} \) 1/4,1/4,0
   \( (1 \ 1/2,1/2,0) \)
6. \( n \) (1/2,1/2,0)
   \( x,y,0 \)
   \( (mz \ 1/2,1/2,0) \)
7. \( a' \) (1/2,0,0)
   \( x,1/4,0 \)
   \( (m'y \ 1/2,1/2,0)' \)
8. \( b' \) (0,1/2,0)
   \( 1/4,y,z \)
   \( (m'z \ 1/2,1/2,0)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) +</td>
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<tr>
<td></td>
<td>(1/2,1/2,0) +</td>
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<tr>
<td>16 r 1 (1) x,y,z [u,v,w]</td>
<td>(2) ( \bar{x},y,\bar{z} [\bar{u},\bar{v},w] )</td>
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<tr>
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<td>(3) ( \bar{x},y,\bar{z} [\bar{u},\bar{v},w] )</td>
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<td>(4) ( x,\bar{y},\bar{z} [\bar{u},\bar{v},w] )</td>
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<td>(5) ( x,\bar{y},\bar{z} [\bar{u},\bar{v},w] )</td>
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<td>(8) ( x,y,z [\bar{u},\bar{v},w] )</td>
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<tr>
<td>8 q ( \ldots m ) x,y,1/2 [0,0,w]</td>
<td>( \bar{x},\bar{y},1/2 [0,0,w] )</td>
</tr>
<tr>
<td>8 p ( \ldots m ) x,y,0 [0,0,w]</td>
<td>( \bar{x},\bar{y},0 [0,0,w] )</td>
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<tr>
<td>8 o ( \ldots m' ) x,0,z [u,0,w]</td>
<td>( \bar{x},0,z [u,0,w] )</td>
</tr>
<tr>
<td>8 n ( \ldots m' ) ( 0,0,z [0,v,w] )</td>
<td>( 0,\bar{y},z [\bar{u},\bar{v},w] )</td>
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<tr>
<td>8 m ( \ldots m' ) ( 1/4,1/4,z [0,0,w] )</td>
<td>( 3/4,1/4,\bar{z} [0,0,w] )</td>
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<tr>
<td>4 l ( m'm'2 ) ( 0,1/2,z [0,0,w] )</td>
<td>( 0,1/2,\bar{z} [0,0,w] )</td>
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<tr>
<td>4 k ( m'm'2 ) ( 0,0,z [0,0,w] )</td>
<td>( 0,0,\bar{z} [0,0,w] )</td>
</tr>
<tr>
<td>4 j ( m'2'm ) ( 0,y,1/2 [0,0,w] )</td>
<td>( 0,\bar{y},1/2 [0,0,w] )</td>
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<tr>
<td>4 i ( m'2'm ) ( 0,y,0 [0,0,w] )</td>
<td>( 0,\bar{y},0 [0,0,w] )</td>
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<tr>
<td>4 h ( 2'm'm ) ( x,0,1/2 [0,0,w] )</td>
<td>( \bar{x},0,1/2 [0,0,w] )</td>
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<td>4 g ( 2'm'm ) ( x,0,0 [0,0,w] )</td>
<td>( \bar{x},0,0 [0,0,w] )</td>
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<tr>
<td>4 f ( \ldots /m ) ( 1/4,1/4,1/2 [0,0,w] )</td>
<td>( 3/4,1/4,1/2 [0,0,w] )</td>
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<tr>
<td>4 e ( \ldots /m ) ( 1/4,1/4,0 [0,0,w] )</td>
<td>( 3/4,1/4,0 [0,0,w] )</td>
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<td>2 d ( m'm'm ) ( 0,0,1/2 [0,0,w] )</td>
<td>( 0,0,1/2 [0,0,w] )</td>
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<tr>
<td>2 c ( m'm'm ) ( 1/2,0,1/2 [0,0,w] )</td>
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<td>2 a ( m'm'm ) ( 0,0,0 [0,0,w] )</td>
<td>( 0,0,0 [0,0,w] )</td>
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</table>

Symmetry of Special Projections
Along [0,0,1]  c2m'm'
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0]  p2'mm'
a* = -c  b* = b/2
Origin at x,0,0

Along [0,1,0]  p2'mm'
a* = c  b* = a/2
Origin at 0,y,0

65.5.549 - 2 - 1089
Cmm'm'    
mm'm'    
Orthorhombic

65.6.550

Origin at center (mm'm')

Asymmetric unit  
0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1       
(1|0,0,0)

(2) 2' 0,0,z
(2_2^z|0,0,0)'

(3) 2' y,0
(2_2^y|0,0,0)'

(4) 2 x,0,0
(2_x|0,0,0)

(5) 1
(1|0,0,0)

(6) m' x,y,0
(m_2^x|0,0,0)'

(7) m' x,0,z
(m_y|0,0,0)'

(8) m 0,y,z
(m_z|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1|1/2,1/2,0)

(2) 2' 1/4,1/4,z
(2_2^z|1/2,1/2,0)'

(3) 2' (0,1/2,0) 1/4,y,0
(2_2^y|1/2,1/2,0)'

(4) 2 (1/2,0,0) x,1/4,0
(2_x|1/2,1/2,0)

(5) ' 1/4,1/2,0
(1|1/2,1/2,0)

(6) m' (1/2,1/2,0) x,y,0
(m_2^x|1/2,1/2,0)'

(7) a' (1/2,0,0) x,1/4,z
(m_y|1/2,1/2,0)'

(8) b (0,1/2,0) 1/4,y,z
(m_z|1/2,1/2,0)

65.6.550 - 1 - 1090
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

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<tr>
<th>Multiplicity</th>
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<tr>
<td>16 r</td>
<td>1 x,y,z [u,v,w]</td>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(4) x,y,z [u,v,w]</td>
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<tr>
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<td>x,0,z [u,v,0]</td>
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<td>0,0,1/2 [u,v,0]</td>
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<tr>
<td>2 c</td>
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<tr>
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<td>0,0,0 [u,v,0]</td>
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<td></td>
<td>0,0,0 [u,v,0]</td>
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</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: c2′mm′
  - **a* = a**
  - **b* = b**
  - Origin at 0,0,z

- **Along [1,0,0]**: p2mm1′
  - **a* = b/2**
  - **b* = c**
  - Origin at x,0,0

- **Along [0,1,0]**: p2′mm′
  - **a* = -a/2**
  - **b* = c**
  - Origin at 0,y,0
Origin at center \((m'm'm')\)

Asymmetric unit \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0) + \) set

\[\begin{align*}
(1) & \quad 1 \\
& \quad (1|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2_z|0,0,0) \\
(5) & \quad T \quad 0,0,0 \\
& \quad (1|0,0,0)' \\
(6) & \quad m' \quad x,y,0 \\
& \quad (m_z|0,0,0)' \\
(7) & \quad m' \quad x,0,z \\
& \quad (m_y|0,0,0)' \\
(8) & \quad m' \quad 0,y,z \\
& \quad (m_x|0,0,0)' \\
\end{align*}\]

For \((1/2,1/2,0) + \) set

\[\begin{align*}
(1) & \quad t \quad (1/2,1/2,0) \\
& \quad (1|1/2,1/2,0) \\
(2) & \quad 2 \quad 1/4,1/4,z \\
& \quad (2_z|1/2,1/2,0) \\
(5) & \quad T \quad 1/4,1/4,0 \\
& \quad (1|1/2,1/2,0)' \\
(6) & \quad n' \quad (1/2,1/2,0) \quad x,y,0 \\
& \quad (m_z|1/2,1/2,0)' \\
(7) & \quad a' \quad (1/2,0,0) \quad x,1/4,z \\
& \quad (m_y|1/2,1/2,0)' \\
(8) & \quad b' \quad (0,1/2,0) \quad 1/4,y,z \\
& \quad (m_x|1/2,1/2,0)' \\
\end{align*}\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1);t(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
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<th>Coordinates</th>
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<tbody>
<tr>
<td>Wyckoff letter, Site Symmetry.</td>
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<td>m'm'm'</td>
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<tr>
<td>2 b</td>
<td>m'm'm'</td>
</tr>
<tr>
<td>2 a</td>
<td>m'm'm'</td>
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</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2m'm'</th>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
<th>Along [0,1,0]</th>
<th>p2m'm'</th>
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</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = b/2)</td>
<td>(b^* = c)</td>
<td>(a^* = c)</td>
<td>(b^* = a/2)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
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<td></td>
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</tr>
</tbody>
</table>
Origin at center (mmm)

Asymmetric unit  

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For \((0,0,0) + \text{set}\):

\[ \begin{align*}
&\text{(1)} \, t \quad (1|0,0,0) \\
&\quad \bar{t} \quad 0,0,0 \\
&\quad m \quad x,y,0 \\
&\quad m' \quad x,0,1/2 \\
&\quad t' \quad (0,0,1) \\
&\quad \bar{t}' \quad 0,0,1/2 \\
&\quad m'' \quad x,y,1/2 \\
&\quad m''' \quad x,0,1/2 \\
&\quad t'' \quad (1/2,1/2,1) \\
&\quad \bar{t}'' \quad 1/4,1/4,1/2 \\
&\quad m''' \quad x,0,1/2 \\
&\quad m''''' \quad x,0,1/2 \\
&\quad t''' \quad (1/2,1/2,1,1) \\
&\quad \bar{t}''' \quad 1/4,1/4,1/2 \\
&\quad m'''''' \quad x,y,1/2 \\
&\quad m''''''' \quad x,0,1/2 \\
&\quad t'''' \quad (1/2,1/2,1,1) \\
&\quad \bar{t}'''' \quad 1/4,1/4,1/2 \\
\end{align*} \]

For \((1/2,1/2,0) + \text{set}\):

\[ \begin{align*}
&\text{(1)} \, t \quad (1/2,1/2,2,0) \\
&\quad \bar{t} \quad 1/4,1/4,0 \\
&\quad m \quad x,y,0 \\
&\quad m' \quad x,0,1/2 \\
&\quad t' \quad (0,0,1) \\
&\quad \bar{t}' \quad 0,0,1/2 \\
&\quad m'' \quad x,y,1/2 \\
&\quad m''' \quad x,0,1/2 \\
&\quad t'' \quad (1/2,1/2,1) \\
&\quad \bar{t}'' \quad 1/4,1/4,1/2 \\
&\quad m''' \quad x,0,1/2 \\
&\quad m''''' \quad x,0,1/2 \\
&\quad t''' \quad (1/2,1/2,1,1) \\
&\quad \bar{t}''' \quad 1/4,1/4,1/2 \\
\end{align*} \]

For \((0,0,1)' + \text{set}\):

\[ \begin{align*}
&\text{(1)} \, t' \quad (1/2,1/2,1) \\
&\quad \bar{t}' \quad 1/4,1/4,1/2 \\
&\quad m' \quad x,y,1/2 \\
&\quad m'' \quad x,0,1/2 \\
&\quad t'' \quad (1/2,1/2,1) \\
&\quad \bar{t}'' \quad 1/4,1/4,1/2 \\
&\quad m''' \quad x,0,1/2 \\
&\quad m''''' \quad x,0,1/2 \\
&\quad t''' \quad (1/2,1/2,1,1) \\
&\quad \bar{t}''' \quad 1/4,1/4,1/2 \\
\end{align*} \]

For \((1/2,1/2,1)' + \text{set}\):

\[ \begin{align*}
&\text{(1)} \, t'' \quad (1/2,1/2,1,1) \\
&\quad \bar{t}'' \quad 1/4,1/4,1/2 \\
&\quad m'' \quad x,y,1/2 \\
&\quad m''' \quad x,0,1/2 \\
&\quad t''' \quad (1/2,1/2,1,1) \\
&\quad \bar{t}''' \quad 1/4,1/4,1/2 \\
&\quad m''' \quad x,0,1/2 \\
&\quad m''''' \quad x,0,1/2 \\
&\quad t''' \quad (1/2,1/2,1,1) \\
&\quad \bar{t}''' \quad 1/4,1/4,1/2 \\
\end{align*} \]
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)*</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
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<tr>
<td>32 r 1</td>
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<td>16 q ..m'</td>
<td>x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
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<tr>
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<td>1/4,1/4,z [0,0,w]</td>
<td>3/4,1/4,z [0,0,w]</td>
<td>3/4,3/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 l mm2</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>8 k mm2</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>8 j m2'm'</td>
<td>0,y,1/2 [u,0,0]</td>
<td>0,y,1/2 [u,0,0]</td>
<td>0,y,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 i m2m</td>
<td>0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
</tr>
<tr>
<td>8 h 2'm'm'</td>
<td>x,0,1/2 [0,v,0]</td>
<td>x,0,1/2 [0,v,0]</td>
<td>x,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 g 2mm</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>8 f ..2/m'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 e ..2/m</td>
<td>1/4,1/4,0 [0,0,w]</td>
<td>3/4,1/4,0 [0,0,w]</td>
<td>3/4,1/4,0 [0,0,w]</td>
</tr>
<tr>
<td>4 d mmm'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c mmm'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b mmm</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a mmm</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
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</thead>
<tbody>
<tr>
<td>c2mm1'</td>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = c</td>
</tr>
<tr>
<td>p2mm1'</td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = b/2</td>
</tr>
<tr>
<td>p2mm1'</td>
<td>a* = a/2</td>
<td>b* = b/2</td>
<td>a* = a/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
Origin at x,0,0
Origin at 0,y,0
Origin at center (mmm)

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. (1 0,0,0)
   (1 0,0,0)

2. (2 0,0,z)
   (2 0,0,0)

3. (3 2 y,0)
   (2 y 0,0,0)

4. (4 2 x,0,0)
   (2 x 0,0,0)

For (1/2,1/2,0) + set

1. (1 1/2,1/2,0)
   (1 1/2,1/2,0)

2. (2 1/4,1/4,z)
   (2 1/2,1/2,0)

3. (3 2 1/1,2,0)
   (2 1/2,1/2,0)

4. (4 2 1/2,1/2,0)
   (2 1/2,1/2,0)

For (1/2,1/2,0) + set

1. (1 1/2,1/2,0)
   (1 1/2,1/2,0)

2. (2 1/4,1/4,z)
   (2 1/2,1/2,0)

3. (3 2 1/1,2,0)
   (2 1/2,1/2,0)

4. (4 2 1/2,1/2,0)
   (2 1/2,1/2,0)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>16 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td>8 q .m</td>
<td>x,y,1/2 [0,0,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 p .m</td>
<td>x,y,0 [0,0,w]</td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 o .m</td>
<td>x,0,z [0,v,0]</td>
<td>(9) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>8 n m..</td>
<td>0,y,z [u,0,0]</td>
<td>(11) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>8 m .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
<td>(13) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(14) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4 l mm2</td>
<td>0,1/2,z [0,0,0]</td>
<td>(15) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 k mm2</td>
<td>0,0,z [0,0,0]</td>
<td>(16) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4 j m2m</td>
<td>0,y,1/2 [0,0,0]</td>
<td>(17) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 i m2m</td>
<td>0,y,0 [0,0,0]</td>
<td>(18) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4 h 2mm</td>
<td>x,0,1/2 [0,0,0]</td>
<td>(19) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 g 2mm</td>
<td>x,0,0 [0,0,0]</td>
<td>(20) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4 f ..2'/m</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>(21) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e ..2'/m</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>(22) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d mmm</td>
<td>0,0,1/2 [0,0,0]</td>
<td>(23) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c mmm</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>(24) x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b mmm</td>
<td>1/2,0,0 [0,0,0]</td>
<td>(25) x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a mmm</td>
<td>0,0,0 [0,0,0]</td>
<td>(26) x,y,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]** c2mm1'  
  \(a^* = a\) \(b^* = b\)  
  Origin at 0,0,z

- **Along [1,0,0]** p2mm1'  
  \(a^* = b/2\) \(b^* = c\)  
  Origin at x,0,0

- **Along [0,1,0]** p2mm1'  
  \(a^* = c\) \(b^* = a/2\)  
  Origin at 0,y,0
Orthorhombic

C\textsubscript{I}mmm

\begin{align*}
65.10.554
\end{align*}

\begin{align*}
\text{Symmetry Operations}
\end{align*}

For \((0,0,0) + \text{set}\):

\begin{align*}
(1) \ 1 & \quad (2) \ z \ \ 0,0,z \\
(1|0,0,0) & \quad (2_z|0,0,0) \\
(5) \overset{\ast}{\text{T}} & \quad (6) \ m \ x,y,0 \\
(\overset{\ast}{\text{T}}|0,0,0) & \quad (m_z|0,0,0)
\end{align*}

For \((1/2,1/2,0)' + \text{set}\):

\begin{align*}
(1) \ t' & \quad (2) \ 2' \ 1/4,1/4,z \\
(1/2,1/2,0)' & \quad (2_2'\mid1/2,1/2,0)' \\
(5) \overset{\text{T}}{\text{T}} & \quad (6) \ n' \ x,y,0 \\
(\overset{\text{T}}{\text{T}}\mid1/2,1/2,0)' & \quad (m_z|1/2,1/2,0)'
\end{align*}

For \((0,0,1)' + \text{set}\):

\begin{align*}
(1) \ t' & \quad (2) \ 2' \ 0,0,z \\
(0,0,1)' & \quad (2_2'|0,0,1)' \\
(5) \overset{\text{T}}{\text{T}} & \quad (6) \ m' \ x,y,1/2 \\
(\overset{\text{T}}{\text{T}}\mid0,0,1)' & \quad (m_z|0,0,1)'
\end{align*}

For \((1/2,1/2,1) + \text{set}\):

\begin{align*}
(1) \ t & \quad (2) \ 2 \ 0,0,1/2 \\
(1/2,1/2,1) & \quad (2_2|1/2,1/2,1) \\
(5) \overset{\text{T}}{\text{T}} & \quad (6) \ n \ x,y,1/2 \\
(\overset{\text{T}}{\text{T}}\mid1/2,1/2,1) & \quad (m_z|1/2,1/2,1)
\end{align*}
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>( (0,0,0) + (0,0,1)' + (1/2,1/2,0)' + (1/2,1/2,1) + (0,0,0) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 r 1</td>
<td>(1) ( x,y,z [u,v,w] )</td>
<td>( (2) \overline{x},y,\overline{z} [\overline{u},v,\overline{w}] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( (3) x,y,\overline{z} [\overline{u},v,\overline{w}] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( (4) x,\overline{y},\overline{z} [u,\overline{v},\overline{w}] )</td>
</tr>
<tr>
<td>16 q .m'</td>
<td>( x,y,1/2 [u,v,0] )</td>
<td>( (2) \overline{x},\overline{y},1/2 [\overline{u},\overline{v},0] )</td>
</tr>
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<td>( (3) x,\overline{y},1/2 [u,\overline{v},0] )</td>
</tr>
<tr>
<td>16 p .m</td>
<td>( x,y,0 [0,0,w] )</td>
<td>( (2) \overline{x},\overline{y},0 [0,0,w] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( (3) x,\overline{y},0 [u,\overline{v},0] )</td>
</tr>
<tr>
<td>16 o .m.</td>
<td>( x,0,z [0,v,0] )</td>
<td>( (2) \overline{x},0,z [\overline{u},v,0] )</td>
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<tr>
<td></td>
<td></td>
<td>( (3) x,0,z [0,0,\overline{w}] )</td>
</tr>
<tr>
<td>16 n m..</td>
<td>( 0,y,z [u,0,0] )</td>
<td>( (2) \overline{0},y,z [\overline{u},0,0] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( (3) 0,y,\overline{z} [u,0,0] )</td>
</tr>
<tr>
<td>16 m ..2'</td>
<td>( 1/4,1/4,z [u,v,0] )</td>
<td>( (2) 3/4,1/4,\overline{z} [u,\overline{v},0] )</td>
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<tr>
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<td>( (3) 3/4,3/4,\overline{z} [u,\overline{v},0] )</td>
</tr>
<tr>
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<td>( 0,1/2,z [0,0,0] )</td>
<td>( (2) 0,1/2,\overline{z} [0,0,0] )</td>
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<tr>
<td>8 k mm2</td>
<td>( 0,0,z [0,0,0] )</td>
<td>( (2) 0,0,\overline{z} [0,0,0] )</td>
</tr>
<tr>
<td>8 j m2m'</td>
<td>( 0,y,1/2 [u,0,0] )</td>
<td>( (2) 0,\overline{y},1/2 [\overline{u},0,0] )</td>
</tr>
<tr>
<td>8 i m2m</td>
<td>( 0,y,0 [0,0,0] )</td>
<td>( (2) 0,\overline{y},0 [0,0,0] )</td>
</tr>
<tr>
<td>8 h 2'mm'</td>
<td>( x,0,1/2 [0,v,0] )</td>
<td>( (2) \overline{x},0,1/2 [0,\overline{v},0] )</td>
</tr>
<tr>
<td>8 g 2mm</td>
<td>( x,0,0 [0,0,0] )</td>
<td>( (2) \overline{x},0,0 [0,0,0] )</td>
</tr>
<tr>
<td>8 f ..2'/m'</td>
<td>( 1/4,1/4,1/2 [u,v,0] )</td>
<td>( (2) 3/4,1/4,1/2 [u,\overline{v},0] )</td>
</tr>
<tr>
<td>8 e ..2'/m</td>
<td>( 1/4,1/4,0 [0,0,0] )</td>
<td>( (2) 3/4,1/4,0 [0,0,0] )</td>
</tr>
<tr>
<td>4 d mm..</td>
<td>( 0,0,1/2 [0,0,0] )</td>
<td>( (2) 0,0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>4 c mm..</td>
<td>( 1/2,0,1/2 [0,0,0] )</td>
<td>( (2) 1/2,0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>4 b mmm</td>
<td>( 1/2,0,0 [0,0,0] )</td>
<td>( (2) 1/2,0,0 [0,0,0] )</td>
</tr>
<tr>
<td>4 a mmm</td>
<td>( 0,0,0 [0,0,0] )</td>
<td>( (2) 0,0,0 [0,0,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\)  c2mm1'  \( a^* = a \)  \( b^* = b \)  Origin at \( 0,0,z \)
- Along \([1,0,0]\)  p2mm1'  \( a^* = b/2 \)  \( b^* = c \)  Origin at \( x,0,0 \)
- Along \([0,1,0]\)  p2mm1'  \( a^* = c \)  \( b^* = a/2 \)  Origin at \( 0,y,0 \)
**Symmetry Operations**

For (0,0,0) + set

1. \( \tau \) (0,0,0)
2. \( 2 \) 0,0,z
3. \( 2' \) 0,y,0
4. \( 2' \) x,0,0
5. \( m' \) x,0,z
6. \( m' \) 0,y,z
7. \( m' \) 0,0,0
8. \( m' \) 0,0,0

For (1/2,1/2,0) + set

1. \( \tau \) (1/2,1/2,0)
2. \( 2 \) 1/4,1/4,z
3. \( 2' \) (0,1/2,0) 1/4,y,0
4. \( 2' \) (1/2,0,0) x,1/4,0
5. \( m' \) x,y,0
6. \( m' \) 1/4,1/4,0
7. \( m' \) 1/4,y,z
8. \( m' \) 1/4,y,z

For (0,0,1) + set

1. \( \tau \) (0,0,1)
2. \( 2' \) (0,0,1) 0,0,z
3. \( 2' \) (0,0,1) 0,0,z
4. \( 2' \) (0,0,1) 0,0,z
5. \( m' \) x,y,1/2
6. \( m' \) 0,0,1/2
7. \( m' \) 0,0,1/2
8. \( m' \) 0,0,1/2

For (1/2,1/2,1) + set

1. \( \tau \) (1/2,1/2,1)
2. \( 2' \) (0,0,1) 1/4,1/4,z
3. \( 2' \) (0,0,1) 1/4,1/4,z
4. \( 2' \) (0,0,1) 1/4,1/4,z
5. \( m' \) x,y,1/2
6. \( m' \) 1/4,1/4,1/2
7. \( m' \) 1/4,1/4,1/2
8. \( m' \) 1/4,1/4,1/2

**Origin at center (m'm'm)**

**Asymmetric unit**

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]
Generators selected: (1); t(1,0,0); t(0,1,0); t'(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,1)' +</td>
</tr>
<tr>
<td>(1/2,1/2,0) +</td>
<td>(1/2,1/2,1)' +</td>
</tr>
</tbody>
</table>

- **32 r 1** (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) x,y,z [u,v,w] (8) x,y,z [u,v,w]

- **16 q ..m'** x,y,1/2 [u,v,0] x,y,1/2 [u,v,0] x,y,1/2 [u,v,0]

- **16 p ..m** x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w]

- **16 o ..m'** x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w]

- **16 n ..m'** 0,y,z [0,v,w] 0,y,z [0,v,w] 0,y,z [0,v,w] 0,y,z [0,v,w]

- **16 m ..2** 1/4,1/4,z [0,0,w] 3/4,1/4,z [0,0,w] 3/4,3/4,z [0,0,w] 1/4,3/4,z [0,0,w]

- **8 l m'm'2** 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w]

- **8 k m'm'2** 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w]

- **8 j m'2m'** 0,y,1/2 [0,v,0] 0,y,1/2 [0,v,0] 0,y,1/2 [0,v,0] 0,y,1/2 [0,v,0]

- **8 i m'2'm** 0,y,0 [0,0,w] 0,y,0 [0,0,w] 0,y,0 [0,0,w] 0,y,0 [0,0,w]

- **8 h 2m'm'** x,0,1/2 [u,0,0] x,0,1/2 [u,0,0] x,0,1/2 [u,0,0] x,0,1/2 [u,0,0]

- **8 g 2'm'm** x,0,0 [0,0,w] x,0,0 [0,0,w] x,0,0 [0,0,w] x,0,0 [0,0,w]

- **8 f ..2'/m'** 1/4,1/4,1/2 [u,v,0] 3/4,1/4,1/2 [u,v,0] 3/4,1/4,1/2 [u,v,0] 3/4,1/4,1/2 [u,v,0]

- **8 e ..2/m** 1/4,1/4,0 [0,0,w] 3/4,1/4,0 [0,0,w] 3/4,1/4,0 [0,0,w] 3/4,1/4,0 [0,0,w]

- **4 d mmm'** 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0]

- **4 c mmm'** 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]

- **4 b m'm'm** 1/2,0,0 [0,0,w] 1/2,0,0 [0,0,w] 1/2,0,0 [0,0,w] 1/2,0,0 [0,0,w]

- **4 a m'm'm** 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,0,0] p2\textsubscript{2}2m'm' Along [0,1,0] p2\textsubscript{2}2mm'  
\textbf{a}^* = \textbf{a} \quad \textbf{b}^* = \textbf{b}  
\textbf{a}^* = -\textbf{c} \quad \textbf{b}^* = \textbf{b}/2  
\textbf{a}^* = \textbf{c} \quad \textbf{b}^* = \textbf{a}/2  
Origin at 0,0,z Origin at x,0,1/4 Origin at 0,y,0
Origin at center (mm'm')

Asymmetric unit
0 < x < 1/4;
0 < y < 1/2;
0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)
(5) t 0,0,0
(1 | 0,0,0)
(6) m' x,y,0
(mz | 0,0,0)

(2) 2' 0,0,z
(2z | 0,0,0)
(7) m' x,0,z
(mz | 0,0,0)

(3) 2' y,0
(2z | 0,0,0)
(8) m 0,y,z
(mz | 0,0,0)

(4) 2 x,0,0
(2z | 0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)
(5) t 1/4,1/4,0
(1 | 1/2,1/2,0)
(6) m' x,y,0
(mz | 0,0,0)

(2) 2' 1/4,1/4,z
(2z | 1/2,1/2,0)
(7) m' x,0,z
(mz | 0,0,0)

(3) 2' (0,1/2,0)
(2z | 1/2,1/2,0)
(8) m 0,y,z
(mz | 0,0,0)

(4) 2 (1/2,0,0)
(2z | 1/2,1/2,0)

For (0,0,1)' + set

(1) t' (0,0,1)
(1 | 0,0,1)
(5) t 0,0,1/2
(1 | 0,0,1)
(6) m x,y,1/2
(mz | 0,0,1)

(2) 2 (0,0,1)
(2z | 0,0,1)
(7) c (0,0,1)
(mz | 0,0,1)

(3) 2 0,y,1/2
(2z | 0,0,1)
(8) c' (0,0,1)
(mz | 0,0,1)

(4) 2' x,0,1/2
(2z | 0,0,1)

For (1/2,1/2,1)' + set

(1) t' (1/2,1/2,1)
(1 | 1/2,1/2,1)
(5) t 1/4,1/4,1/2
(1 | 1/2,1/2,1)
(6) m (1/2,1/2,0)
(mz | 1/2,1/2,1)

(2) 2 (0,0,1)
(2z | 1/2,1/2,1)
(7) c (1/2,0,1)
(mz | 1/2,1/2,1)

(3) 2 (0,1/2,0)
(2z | 1/2,1/2,1)
(8) n' (0,1/2,1)
(mz | 1/2,1/2,1)

(4) 2' (1/2,0,0)
(2z | 1/2,1/2,1)'
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' + (1/2,1/2,0) + (1/2,1/2,1)' +</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>(0,0,0) + (0,0,1)' + (1/2,1/2,0) + (1/2,1/2,1)' +</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
</tbody>
</table>

32 r 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) x,y,z [u,v,w] (8) x,y,z [u,v,w]

16 q ..m x,y,1/2 [0,0,w] x,y,1/2 [0,0,w] x,y,1/2 [0,0,w] x,y,1/2 [0,0,w] x,y,1/2 [0,0,w] x,y,1/2 [0,0,w] x,y,1/2 [0,0,w] x,y,1/2 [0,0,w]

16 p ..m' x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0]

16 o ..m' x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w]

16 n m.. 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0]

16 m ..' 1/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0]

8 l mm'2' 0,1/2,z [u,0,0] 0,1/2,z [u,0,0] 0,1/2,z [u,0,0] 0,1/2,z [u,0,0] 0,1/2,z [u,0,0] 0,1/2,z [u,0,0] 0,1/2,z [u,0,0] 0,1/2,z [u,0,0]

8 k mm'2' 0,0,z [u,0,0] 0,0,z [u,0,0] 0,0,z [u,0,0] 0,0,z [u,0,0] 0,0,z [u,0,0] 0,0,z [u,0,0] 0,0,z [u,0,0] 0,0,z [u,0,0]

8 j m2m 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0] 0,y,1/2 [0,0,0]

8 i m2m' 0,y,0 [u,0,0] 0,y,0 [u,0,0] 0,y,0 [u,0,0] 0,y,0 [u,0,0] 0,y,0 [u,0,0] 0,y,0 [u,0,0] 0,y,0 [u,0,0] 0,y,0 [u,0,0]

8 h 2'm'm x,0,1/2 [0,0,w] x,0,1/2 [0,0,w] x,0,1/2 [0,0,w] x,0,1/2 [0,0,w] x,0,1/2 [0,0,w] x,0,1/2 [0,0,w] x,0,1/2 [0,0,w] x,0,1/2 [0,0,w]

8 g 2'm'm' x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0]

8 f ..'2/m 1/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0]

8 e ..'2/m' 1/4,1/4,0 [u,v,0] 3/4,1/4,0 [u,v,0] 3/4,1/4,0 [u,v,0] 3/4,1/4,0 [u,v,0] 3/4,1/4,0 [u,v,0] 3/4,1/4,0 [u,v,0] 3/4,1/4,0 [u,v,0] 3/4,1/4,0 [u,v,0]

4 d mm'm 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0]

4 c mm'm 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]

4 b mm'm' 1/2,0,0 [u,0,0] 1/2,0,0 [u,0,0] 1/2,0,0 [u,0,0] 1/2,0,0 [u,0,0] 1/2,0,0 [u,0,0] 1/2,0,0 [u,0,0] 1/2,0,0 [u,0,0] 1/2,0,0 [u,0,0]

4 a mm'm' 0,0,0 [u,0,0] 0,0,0 [u,0,0] 0,0,0 [u,0,0] 0,0,0 [u,0,0] 0,0,0 [u,0,0] 0,0,0 [u,0,0] 0,0,0 [u,0,0] 0,0,0 [u,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [0,1,0]</th>
<th>p2e-2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b/2 b* = c</td>
<td>a* = c b* = a/2</td>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 1/2,y,0</td>
</tr>
</tbody>
</table>
Origin at center (m'mm)

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. \( \overline{1} \)
   \((0,0,0)\)

2. \( 2\)
   \((0,0,z)\)

3. \( 2\)
   \((0,y,0)\)

4. \( 2\)
   \((x,0,0)\)

5. \( m\)
   \((x,y,0)\)

6. \( m\)
   \((y,x,0)\)

7. \( m\)
   \((y,0,z)\)

8. \( m\)
   \((0,y,z)\)

For \((1/2,1/2,0)\) + set

1. \( t\)
   \((1/2,1/2,0)\)

2. \( 2\)
   \((1/2,1/4,1/4,z)\)

3. \( 2\)
   \((1/2,1/2,1/4,y,0)\)

4. \( 2\)
   \((1/2,1/2,1/4,x,0)\)

5. \( n\)
   \((1/2,1/4,1/4,0)\)

6. \( n\)
   \((1/2,1/4,1/4,x,0)\)

7. \( a\)
   \((1/2,1/4,1/4,y,0)\)

8. \( b\)
   \((1/2,1/4,1/4,z,0)\)
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5). \)

### Positions

<table>
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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 r 1 ( (1) x,y,z [u,v,w] )  ( (1/2,1/2,0)' + ) ( (0,0,0) + )</td>
<td>( (2) \bar{x},\bar{y},\bar{z} [u\bar{v},w] ) ( (3) x, y, z [u,\bar{v},w] ) ( (4) x, y, z [u,v,w] )</td>
</tr>
<tr>
<td>8 q ..m ( x,y,1/2 [0,0,w] )</td>
<td>( \bar{x}, \bar{y}, 1/2 [0,0,\bar{w}] ) ( x,y,1/2 [0,0,\bar{w}] ) ( x,y,1/2 [0,0,\bar{w}] )</td>
</tr>
<tr>
<td>8 p ..m ( x,y,0 [0,0,w] )</td>
<td>( \bar{x}, \bar{y}, 0 [0,0,\bar{w}] ) ( x,y,0 [0,0,\bar{w}] ) ( x,y,0 [0,0,\bar{w}] )</td>
</tr>
<tr>
<td>8 o ..m ( x,0,z [0,v,0] )</td>
<td>( \bar{x}, 0, z [0,v,\bar{0}] ) ( x, 0, z [0,\bar{v},0] ) ( x,0,\bar{z} [0,\bar{v},0] )</td>
</tr>
<tr>
<td>8 n m'.. 0,y,z [0,v,w]</td>
<td>( 0, y, z [0, v, \bar{w}] ) ( 0, y, \bar{z} [0, v, \bar{w}] ) ( 0, y, \bar{z} [0, v, \bar{w}] )</td>
</tr>
<tr>
<td>8 m ..2 ( 1/4,1/4,z [0,0,w] )</td>
<td>( 3/4,1/4, \bar{z} [0,0,\bar{w}] ) ( 3/4,3/4, \bar{z} [0,0,\bar{w}] ) ( 1/4,3/4, z [0,0,\bar{w}] )</td>
</tr>
<tr>
<td>4 l m'm'2' ( 0,1/2, z [0,v,0] )</td>
<td>( 0,1/2, z [0,v,0] ) ( 0,1/2, z [0,v,0] )</td>
</tr>
<tr>
<td>4 k m'm'2' ( 0,0, z [0,v,0] )</td>
<td>( 0,0, \bar{z} [0,\bar{v},0] ) ( 0,0, \bar{z} [0,\bar{v},0] )</td>
</tr>
<tr>
<td>4 j m'2'm ( 0, y,1/2 [0,0,w] )</td>
<td>( 0, y,1/2 [0,0,w] ) ( 0, \bar{y}, 1/2 [0,0,\bar{w}] )</td>
</tr>
<tr>
<td>4 i m'2'm ( 0, y,0 [0,0,w] )</td>
<td>( 0, y,0 [0,0,\bar{w}] ) ( 0, \bar{y}, 0 [0,0,\bar{w}] )</td>
</tr>
<tr>
<td>4 h 2mm ( x,0,1/2 [0,0,0] )</td>
<td>( \bar{x}, 0,1/2 [0,0,0] ) ( \bar{x}, 0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>4 g 2mm ( x,0,0 [0,0,0] )</td>
<td>( \bar{x}, 0,0 [0,0,0] ) ( x,0,0 [0,0,0] )</td>
</tr>
<tr>
<td>4 f ..2/m ( 1/4,1/4,1/2 [0,0,w] )</td>
<td>( 3/4,1/4,1/2 [0,0,w] ) ( 3/4,1/4,1/2 [0,0,w] )</td>
</tr>
<tr>
<td>4 e ..2/m ( 1/4,1/4,0 [0,0,w] )</td>
<td>( 3/4,1/4,0 [0,0,w] ) ( 3/4,1/4,0 [0,0,w] )</td>
</tr>
<tr>
<td>2 d m'm'm ( 0,0,1/2 [0,0,0] )</td>
<td>( 0,0,1/2 [0,0,0] ) ( 0,0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>2 c m'm'm ( 1/2,0,1/2 [0,0,0] )</td>
<td>( 1/2,0,1/2 [0,0,0] ) ( 1/2,0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>2 b m'm'm ( 1/2,0,0 [0,0,0] )</td>
<td>( 1/2,0,0 [0,0,0] ) ( 1/2,0,0 [0,0,0] )</td>
</tr>
<tr>
<td>2 a m'm'm ( 0,0,0 [0,0,0] )</td>
<td>( 0,0,0 [0,0,0] ) ( 0,0,0 [0,0,0] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along** \([0,0,1]\) \( \text{c2mm}^1 \)
- **Along** \([1,0,0]\) \( \text{p}_{2\alpha z}^z 2\text{mm} \)
- **Along** \([0,1,0]\) \( \text{p}2\text{mm} 1' \)

\( \mathbf{a}^* = \mathbf{a} \) \( \mathbf{b}^* = \mathbf{b} \)

- Origin at \(0,0,z\)

\( \mathbf{a}^* = \mathbf{b}/2 \) \( \mathbf{b}^* = \mathbf{c} \)

- Origin at \(x,0,0\)

\( \mathbf{a}^* = \mathbf{c} \) \( \mathbf{b}^* = \mathbf{a}/2 \)

- Origin at \(0,y,0\)
Orthorhombic

Origin at center (mmm')

Asymmetric unit  
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2' 0,0,z
(2) 2' 0,0,0

(3) 2' 0,y,0
(3) 2' 0,0,0

(4) 2' x,0,0
(4) 2' x,0,0

(5) 1/4,1/4,0
(5) 1/4,1/4,0

(6) m' x,y,0
(6) m' 0,0,0

(7) m 0,x,z
(7) m 0,0,0

(8) m 0,y,z
(8) m 0,0,0

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(1) 1/2,1/2,0

(2) 2' 1/4,1/4,z
(2) 2' 1/2,1/2,0

(3) 2 (0,1/2,0) 1/4,y,0
(3) 2 (0,1/2,0) 1/2,1/2,0

(4) 2 (1/2,0,0) x,1/4,0
(4) 2 (1/2,0,0) x,1/2,1/2,0

(5) 1/4,1/4,0
(5) 1/2,1/2,0

(6) n (1/2,1/2,0) x,y,0
(6) n (1/2,1/2,0)

(7) a' (1/2,0,0) x,1/4,z
(7) a' (1/2,0,0) 1/2,1/2,0

(8) b' (0,1/2,0) 1/4,y,z
(8) b' (0,1/2,0) 1/2,1/2,0

65.14.558-1 - 1106
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0)’ +</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>16 r 1</th>
<th>(1) x,y,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5) x,y,z [u,v,w]</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>8 q .m’</th>
<th>x,y,1/2 [u,v,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 p .m’</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 o .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 n .m.</td>
<td>0,y,z [u,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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<th>1/4,1/4,z [u,v,0]</th>
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</thead>
<tbody>
<tr>
<td>4 l mm2</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 k mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 j m2’m’</td>
<td>0,y,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 i m2’m’</td>
<td>0,y,0 [u,0,0]</td>
</tr>
<tr>
<td>4 h 2’m’m’</td>
<td>x,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 g 2’m’m’</td>
<td>x,0,0 [0,v,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4 f .2’/m’</th>
<th>1/4,1/4,1/2 [u,v,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e .2’/m’</td>
<td>1/4,1/4,0 [u,v,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2 d mmm’</th>
<th>0,0,1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 c mmm’</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b mmm’</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a mmm’</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( c_{p,2mm} \)
\( a^* = a \) \( b^* = b \)
Origin at 0,0,z

Along [1,0,0] \( p2mm1' \)
\( a^* = b/2 \) \( b^* = c \)
Origin at x,0,0

Along [0,1,0] \( p2mm1' \)
\( a^* = c \) \( b^* = a/2 \)
Origin at 0,y,0
Cp\textsuperscript{m'm'm}  

Cp\textsuperscript{2'/m'2'/m'2/m}  

Orthorhombic  

65.15.559  

Orthorhombic  

65.15.559  

Origin at center (m'm'm)  

Asymmetric unit  

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2  

Symmetry Operations  

For (0,0,0) + set  

(1) 1  

(2) 2 0,0,z  

(3) 2' 0,y,0  

(4) 2' x,0,0  

(5) m 0,0,0  

(6) m' x,y,0  

(7) m' x,0,z  

(8) m' 0,y,z  

For (1/2,1/2,0)' + set  

(1) t' (1/2,1/2,0)  

(2) 2' 1/4,1/4,z  

(3) 2 (0,1/2,0) 1/4,y,0  

(4) 2 (1/2,0,0) x,1/4,0  

(5) t' 1/4,1/4,0  

(6) n' (1/2,1/2,0) x,y,0  

(7) a (1/2,0,0) x,1/4,z  

(8) b (0,1/2,0) 1/4,y,z  

65.15.559 - 1 - 1108
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0)' + (2) (3) (5).</td>
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</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 r 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(8) x,y,z [u,v,w]</td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 q 1/4,1/4,z [u,v,0]</td>
<td>3/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>4 l m'm'2 0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 k m'm'2 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 i m'2m 0,y,1/2 [0,0,w]</td>
<td>0,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 i m'2m 0,y,1/2 [0,0,w]</td>
<td>0,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 h 2m'm' x,0,1/2 [0,0,w]</td>
<td>x,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 g 2m'm' x,0,0 [0,0,w]</td>
<td>x,0,0 [0,0,w]</td>
</tr>
<tr>
<td>4 f 1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e 1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d m'm'm 0,0,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 c m'm'm 1/2,0,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b m'm'm 1/2,0,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 a m'm'm 0,0,0 [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1] c2mm1' 
Along [1,0,0] p_{2a*}2mm 
Along [0,1,0] p_{2a*}2mm 

a* = a  
b* = b  
Origin at 0,0,z 

a* = b/2  
b* = c  
Origin at x,1/4,0 

a* = -a/2  
b* = c  
Origin at 0,y,1/4 

---

Continued

65.15.559 - 2 - 1109
Origin at center (mm'm')

Asymmetric unit  
0 ≤ x ≤ 1/4;  
0 ≤ y ≤ 1/2;  
0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1)  
(1|0,0,0)
(2) 2' 0,0,z  
(2|0,0,0)'  
(3) 2' 0,y,0  
(2|0,0,0)'  
(4) 2 0,0  
(2|0,0,0)

(5)  
(1|0,0,0)  
(6) m' x,y,0  
(m|0,0,0)'  
(7) m' x,0,z  
(m|0,0,0)'  
(8) m 0,y,z  
(m|0,0,0)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)  
(1|1/2,1/2,0)'
(2) 2 1/4,1/4,z  
(2|1/2,1/2,0)  
(3) 2 (0,1/2,0)  
(2|1/2,1/2,0)  
(4) 2' (1/2,0,0)  
(2|1/2,1/2,0)'

(5)  
(1|1/2,1/2,0)  
(6) n (1/2,1/2,0)  
(m|1/2,1/2,0)  
(7) a (1/2,0,0)  
(m|1/2,1/2,0)  
(8) b' (0,1/2,0)  
(m|1/2,1/2,0)'

65.16.560 - 1 - 1110
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0)</td>
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<tr>
<td>16 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>8 q ..m'</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 p ..m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 o ..m'</td>
<td>x,0,z [u,0,]</td>
</tr>
<tr>
<td>8 n m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 m ..2</td>
<td>1/4,1/4,z [0,0,]</td>
</tr>
<tr>
<td>4 l mm'2'</td>
<td>0,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>4 k mm'2'</td>
<td>0,0,z [u,0,0]</td>
</tr>
<tr>
<td>4 j m2m'</td>
<td>0,y,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 i m2m'</td>
<td>0,y,0 [u,0,0]</td>
</tr>
<tr>
<td>4 h 2m'm'</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 g 2m'm'</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>4 f ..2/m'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e ..2/m'</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d mm'm'</td>
<td>0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 c mm'm'</td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 b mm'm'</td>
<td>1/2,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2 a mm'm'</td>
<td>0,0,0 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_p,2mm
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2mm1'
a* = b/2  b* = c
Origin at x,0,0

Along [0,1,0] p2221'
a* = -a/2  b* = c
Origin at y,0,0
Cp m'm'm'
65.17.561

mmm1'
Cp 2/m'2/m'2/m'

Orthorhombic

Origin at center (m'm'm')

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2|0,0,0)

(3) 2 0,y,0
(2|0,0,0)

(4) 2 x,0,0
(2|0,0,0)

(5) 1/4,1/4,0
(1/2,1/2,0)

(6) m' x,y,0
(m'z|0,0,0)

(7) m' x,0,z
(m'y|0,0,0)

(8) m' 0,y,z
(m'z|0,0,0)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(1|1/2,1/2,0')

(2) 2' 1/4,1/4,z
(2'|1/2,1/2,0')

(3) 2' (0,1/2,0) 1/4,y,0
(2'|1/2,1/2,0')

(4) 2' (1/2,0,0) x,1/4,0
(2'|1/2,1/2,0')

(5) 1/4,1/4,0
(1|1/2,1/2,0)

(6) n (1/2,1/2,0) x,y,0
(nz|1/2,1/2,0)

(7) a (1/2,0,0)  x,1/4,z
(n|1/2,1/2,0)

(8) b (0,1/2,0)  1/4,y,z
(nz|1/2,1/2,0)
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(5) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
<td>(7) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(8) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 q .m'</td>
<td>x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 p .m'</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 o .m'</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>8 n .m'</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 m .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
<td>3/4,1/4,z [u,v,0]</td>
<td>1/4,3/4,z [u,v,0]</td>
</tr>
<tr>
<td>4 l m'2</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 k m'2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 j m'2m'</td>
<td>0,y,1/2 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 i m'2m'</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 h 2m'm'</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 g 2m'm'</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>4 f .2'/m'</td>
<td>1/4,1/4,1/2 [u,v,0]</td>
<td>3/4,1/4,1/2 [u,v,0]</td>
<td>3/4,1/4,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 e .2'/m'</td>
<td>1/4,1/4,0 [u,v,0]</td>
<td>3/4,1/4,0 [u,v,0]</td>
<td>3/4,1/4,0 [u,v,0]</td>
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<tr>
<td>2 d m'm'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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<td>2 c m'm'</td>
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<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b m'm'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a m'm'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1]  \( c_{p} \cdot 2m'm' \)
- Along [1,0,0]  \( p_{2a} \cdot 2m'm' \)
- Along [0,1,0]  \( p_{2g} \cdot 2m'm' \)

\( a^* = a \quad b^* = b \)

Origin at 0,0,z

\( a^* = b/2 \quad b^* = c \)

Origin at x,0,0

\( a^* = -a/2 \quad b^* = c \)

Origin at 0,y,0
Cm'm'm
65.18.562

Orthorhombic

mmm1'
C2/m'2'/m2'/m

Origin at center (m'mm)

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)
(2) 2' 0,0,z
(2' | 0,0,0)
(3) 2' 0,y,0
(2' | 0,0,0)
(4) 2 x,0,0
(2 | 0,0,0)

(5) T' 0,0,0
(T | 0,0,0)
(6) m x,y,0
(mz | 0,0,0)
(7) m x,0,z
(mz | 0,0,0)
(8) m' 0,y,z
(mz | 0,0,0)

For (1/2,1/2,0)' + set

(1) T' (1/2,1/2,0)
(1 | 1/2,1/2,0)
(2) 2 1/4,1/4,z
(2' | 1/2,1/2,0)
(3) 2 (0,1/2,0) 1/4,y,0
(2 | 1/2,1/2,0)
(4) 2' (1/2,0,0) x,1/4,0
(2 | 1/2,1/2,0)

(5) T 1/4,1/4,0
(T | 1/2,1/2,0)
(6) n' (1/2,1/2,0) x,y,0
(mz' | 1/2,1/2,0)
(7) a' (1/2,0,0) x,1/4,z
(mz | 1/2,1/2,0)
(8) b (0,1/2,0) 1/4,y,z
(mz | 1/2,1/2,0)

For (0,0,1)' + set

(1) T' (0,0,1)
(1 | 0,0,1)
(2) 2 (0,0,1) 0,0,z
(2' | 0,0,1)
(3) 2 0,y,1/2
(2 | 0,0,1)
(4) 2' x,0,1/2
(2 | 0,0,1)

(5) T 0,0,1/2
(T | 0,0,1)
(6) m' x,y,1/2
(mz | 0,0,1)
(7) c' (0,0,1) x,0,z
(mz | 0,0,1)
(8) c (0,0,1) 0,y,z
(mz | 0,0,1)

For (1/2,1/2,1) + set

(1) T (1/2,1/2,1)
(1 | 1/2,1/2,1)
(2) 2' (0,0,1) 1/4,1/4,z
(2' | 1/2,1/2,1)
(3) 2' (0,1/2,0) 1/4,y,1/2
(2 | 1/2,1/2,1)
(4) 2 (1/2,0,0) x,1/4,1/2
(2 | 1/2,1/2,1)

(5) T' 1/4,1/4,1/2
(T | 1/2,1/2,1)
(6) n (1/2,1/2,0) x,y,1/2
(mz | 1/2,1/2,1)
(7) n (1/2,0,1) x,1/4,z
(mz | 1/2,1/2,1)
(8) n' (0,1/2,1) 1/4,y,z
(mz | 1/2,1/2,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,1)' +</td>
<td>1/2,1/2,0) +</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>32 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 q ..m'</td>
<td>x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>16 p ..m</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>16 o ..m.</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>16 n m'..</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>16 m ..2</td>
<td>1/4,1/4,z [0,0,w]</td>
<td>3/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 l m'm'2'</td>
<td>0,1/2,z [0,v,0]</td>
<td>0,1/2,z [0,v,0]</td>
</tr>
<tr>
<td>8 k m'm'2'</td>
<td>0,0,z [0,v,0]</td>
<td>0,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 j m'2m'1'</td>
<td>0,y,1/2 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 i m'2'm</td>
<td>0,y,0 [0,0,w]</td>
<td>0,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 h 2'mm'</td>
<td>x,0,1/2 [0,v,0]</td>
<td>x,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 g 2mm</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>8 f ..2'\m</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 e ..2'\m</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 d m'm'm'</td>
<td>0,0,1/2 [0,v,0]</td>
<td>0,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 c m'm'm'</td>
<td>1/2,0,1/2 [0,v,0]</td>
<td>1/2,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 b m'mm</td>
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<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a m'nm</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1]  c2mm1'
- Along [1,0,0]  p_{c2}mm
- Along [0,1,0]  p2mm1'

\[ \mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b} \]

Origin at 0,0,z
Orthorhombic

Origin at center \((m'm'm)\)

Asymmetric unit

\[0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}\]

Symmetry Operations

For \((0,0,0)\) + set

1. \(T\)
   \((1,0,0,0)\)

2. \(S\)
   \((2_z,0,0,0)\)

3. \(S'\)
   \((0,y,0)\)

4. \(S'\)
   \((x,0,0)\)

5. \(\overline{T}\)
   \((0,0,0)\)

6. \(m\)
   \((x,y,0)\)

7. \(m'\)
   \((x,0,z)\)

8. \(m'\)
   \((0,y,z)\)

For \((1/2,1/2,0)\)' + set

1. \(T'\)
   \((1/2,1/2,2,0)\)

2. \(S'\)
   \((1/4,1/4,z)\)

3. \(S'\)
   \((0,1/2,0)\)

4. \(S'\)
   \((1/2,0,0)\)

5. \(\overline{T}\)
   \((1/2,1/2,0)\)

6. \(n'\)
   \((x,y,0)\)

7. \(a\)
   \((1/2,0,0)\)

8. \(n'\)
   \((0,1/2,0)\)

For \((0,0,1)\)' + set

1. \(T'\)
   \((0,0,1)\)

2. \(S'\)
   \((0,0,1)\)

3. \(S'\)
   \((0,y,1/2)\)

4. \(S'\)
   \((x,0,1/2)\)

5. \(\overline{T}\)
   \((0,0,1)\)

6. \(m'\)
   \((x,y,1/2)\)

7. \(c\)
   \((0,0,1)\)

8. \(c\)
   \((0,0,1)\)

For \((1/2,1/2,1)\) + set

1. \(T\)
   \((1/2,1/2,2,1)\)

2. \(S\)
   \((1/4,1/4,z)\)

3. \(S'\)
   \((0,1/2,0)\)

4. \(S'\)
   \((1/2,0,0)\)

5. \(\overline{T}\)
   \((1/2,1/2,2,1)\)

6. \(n\)
   \((1/2,1/2,0)\)

7. \(n'\)
   \((1/2,0,1)\)

8. \(n'\)
   \((0,1/2,1)\)
Generators selected: (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0) +</td>
<td>(0,0,0)</td>
<td>(1/2,1/2,0)</td>
</tr>
<tr>
<td>(0,0,1)'</td>
<td></td>
<td>(1/2,1/2,1)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 q ..m'</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>16 p ..m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>16 o ..m'..</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>16 n ..m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>16 m ..2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>8 l m'm'2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 k m'm'2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 j m'2m'</td>
<td>0,y,1/2 [0,0,v]</td>
</tr>
<tr>
<td>8 i m'2m'</td>
<td>0,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 h 2m'm'</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 g 2m'm'</td>
<td>x,0,0 [0,0,w]</td>
</tr>
<tr>
<td>8 f ..2'/m'</td>
<td>1/4,1/4,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 e ..2'/m'</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 d m'm'm'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c m'm'm'</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b m'm'm'</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>4 a m'm'm'</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: c2mm1'
  - $a^* = a$, $b^* = b$
  - Origin at 0,0,z

- **Along [1,0,0]**: $p_{2a}$-2mm
  - $a^* = b/2$, $b^* = c$
  - Origin at x,1/4,0

- **Along [0,1,0]**: $p_{2a}$-2mm
  - $a^* = c$, $b^* = a/2$
  - Origin at 1/4,y,0
Origin at center (2/m) at cc2/m

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. \( (1) 1 (0,0,0) \)
2. \( (2) 2 0,0,z (0,0,0) \)
3. \( (3) 2 y,0,1/4 (0,0,1/2) \)
4. \( (4) 2 x,0,1/4 (0,0,1/2) \)
5. \( (5) 1 0,0,0 \)
6. \( (6) m x,y,0 (0,0,0) \)
7. \( (7) c (0,0,1/2) x,0,z (0,0,1/2) \)
8. \( (8) c (0,0,1/2) 0,y,z (0,0,1/2) \)

For (1/2,1/2,0) + set

1. \( (1) t (1/2,1/2,0) \)
2. \( (2) 2 1/4,1/4,z (1/2,1/2,0) \)
3. \( (3) 2 (0,1/2,0) 1/4,y,1/4 (1/2,1/2,1/2) \)
4. \( (4) 2 (1/2,0,0) x,1/4,1/4 (1/2,1/2,1/2) \)
5. \( (5) 1/2,1/2,0 \)
6. \( (6) n (1/2,1/2,0) x,y,0 (1/2,1/2,0) \)
7. \( (7) n (1/2,0,1/2) x,1/4,z (1/2,1/2,1/2) \)
8. \( (8) n (0,1/2,1/2) 1/4,y,z (1/2,1/2,1/2) \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 m</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(3) x, y, z +1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(4) x, y, z +1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(6) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(7) x, y, z +1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(8) x, y, z +1/2 [u, v, w]</td>
</tr>
</tbody>
</table>

| 8 l          | x, y, 0 [0, 0, w]             |
|              | x, y, 1/2 [0, 0, w]           |
|              | x, y, 1/2 [0, 0, w]           |

| 8 k          | 1/4, 1/4, z [0, 0, w]         |
|              | 3/4, 1/4, z +1/2 [0, 0, w]    |
|              | 3/4, 3/4, z [0, 0, w]         |
|              | 1/4, 3/4, z +1/2 [0, 0, w]    |

| 8 j          | 0,1/2, z [0, 0, w]            |
|              | 0,1/2, z [0, 0, w]            |
|              | 0,1/2, z [0, 0, w]            |

| 8 i          | 0,0, z [0, 0, w]              |
|              | 0,0, z [0, 0, w]              |
|              | 0,0, z [0, 0, w]              |

| 8 h          | 0, y, 1/4 [0, v, 0]           |
|              | 0, y, 3/4 [0, v, 0]           |
|              | 0, y, 3/4 [0, v, 0]           |

| 8 g          | x, 0, 1/4 [u, 0, 0]           |
|              | x, 0, 1/4 [u, 0, 0]           |
|              | x, 0, 1/4 [u, 0, 0]           |

| 4 f          | 1/4, 3/4, 0 [0, 0, w]         |
|              | 3/4, 3/4, 1/2 [0, 0, w]       |
|              | 3/4, 3/4, 1/2 [0, 0, w]       |

| 4 e          | 1/4, 1/4, 0 [0, 0, w]         |
|              | 3/4, 1/4, 1/2 [0, 0, w]       |
|              | 3/4, 1/4, 1/2 [0, 0, w]       |

| 4 d          | 0, 1/2, 0 [0, 0, w]           |
|              | 0, 1/2, 1/2 [0, 0, w]         |
|              | 0, 1/2, 1/2 [0, 0, w]         |

| 4 c          | 0, 0, 0 [0, 0, w]             |
|              | 0, 0, 1/2 [0, 0, w]           |
|              | 0, 0, 1/2 [0, 0, w]           |

| 4 b          | 0, 1/2, 1/4 [0, 0, 0]         |
|              | 0, 1/2, 3/4 [0, 0, 0]         |
|              | 0, 1/2, 3/4 [0, 0, 0]         |

| 4 a          | 0, 0, 1/4 [0, 0, 0]           |
|              | 0, 0, 3/4 [0, 0, 0]           |
|              | 0, 0, 3/4 [0, 0, 0]           |

**Symmetry of Special Projections**

- Along [0,0,1]  c2mm1'  
- Along [1,0,0]  p2a2m'  
- Along [0,1,0]  p2a2m'  

\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  
Origin at 0,0,z  

\[ \mathbf{a}^* = -c/2 \quad \mathbf{b}^* = b/2 \]  
Origin at x,0,0  

\[ \mathbf{a}^* = c/2 \quad \mathbf{b}^* = a/2 \]  
Origin at x,0,0
**Symmetry Operations**

For $(0,0,0) +$ set

1. $T (0,0,0)$
2. $2 (0,0,z)$
3. $2 (0,y,1/4)$
4. $2 (x,0,1/4)$
5. $T (1/2,1/2,0)$
6. $n (1/2,1/2,0)$
7. $n (0,1/2,0)$
8. $n (0,0,1/2)$

For $(1/2,1/2,0) +$ set

1. $T (1/2,1/2,0)$
2. $2 (1/2,1/2,0)$
3. $2 (0,1/2,0)$
4. $2 (1/2,0,0)$
5. $T (1/2,1/2,0)$
6. $n (1/2,1/2,0)$
7. $n (0,1/2,0)$
8. $n (0,0,1/2)$

For $(0,0,0)' +$ set

1. $T (0,0,0)'$
2. $2 (0,0,z)'$
3. $2 (0,y,1/4)'$
4. $2 (x,0,1/4)'$
5. $T (0,0,0)'$
6. $m (0,0,z)'$
7. $c' (0,0,1/2) x,0,z$
8. $c' (0,0,1/2) 0,y,z$

For $(1/2,1/2,0)' +$ set

1. $T (1/2,1/2,0)'$
2. $2 (1/2,1/2,0)'$
3. $2 (0,1/2,0)'$
4. $2 (1/2,0,0)'$
5. $T (1/2,1/2,0)'$
6. $n' (1/2,1/2,0)'$
7. $n' (1/2,0,1/2)'$
8. $n' (0,1/2,1/2)'$

**Origin** at center (2/m1') at cc2/m1'

**Asymmetric unit**

$0 \leq x \leq 1/4; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 m 11' (1) x,y,z [0,0,0]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>(5) x,y,z, [0,0,0]</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 l .m1' x,y,0 [0,0,0]</td>
<td>(0,0,0)' +</td>
</tr>
<tr>
<td>8 k .21' 1/4,1/4,z [0,0,0]</td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td>8 j .21' 0,1/2,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>8 i .21' 0,0,z [0,0,0]</td>
<td>(3) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 h .21' 0,y,1/4 [0,0,0]</td>
<td>(4) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 g .21' x,0,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 f .2/m1' 1/4,3/4,0 [0,0,0]</td>
<td>3/4,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e .2/m1' 1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 d .2/m1' 0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2/m1' 0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2221' 0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2221' 0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
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</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [0,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c/2</td>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0

---

66.2.565 - 2 - 1121
Origin at center \((2'/m)\) at \(c'c2'/m\)

Asymmetric unit \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0) + \) set

\begin{align*}
(1) & \quad \text{I} \\
(2') & \quad 0,0,z \\
(2) & \quad 2',0,0,0' \\
(3) & \quad 2',0,y,1/4 \\
(4) & \quad 2',x,0,1/4 \\
(5) & \quad 1/2,1/2,0 \\
(6) & \quad m,x,y,0 \\
(7) & \quad c,0,0,1/2 \\
(8) & \quad c',0,0,1/2' \\
(1') & \quad 0,0,0 \\
(2') & \quad 0,0,0' \\
(6') & \quad m,z,0,0,0 \\
(7') & \quad m,y,0,0,0' \\
(8') & \quad m',0,0,0' \\
\end{align*}

For \((1/2,1/2,0) + \) set

\begin{align*}
(1) & \quad t,1/2,1/2,0 \\
(2') & \quad 1/4,1/4,0 \\
(2) & \quad 2',1/2,1/2,0' \\
(3) & \quad 2',0,1/2,0 \\
(4) & \quad 2',x,0,1/4 \\
(5) & \quad 1/4,1/4,0 \\
(6) & \quad n,1/2,1/2,0 \\
(7) & \quad n,1/2,0,1/2 \\
(8) & \quad n',0,1/2,1/2' \\
(1') & \quad 1/2,1/2,0 \\
(2') & \quad 1/2,1/2,0' \\
(6') & \quad m,z,1/2,1/2,0 \\
(7') & \quad m,y,1/2,1/2,0 \\
(8') & \quad m',1/2,1/2,1/2' \\
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>16 m</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 l</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 k</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,z [u,v,0]</td>
</tr>
<tr>
<td>8 j</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [u,0,0]</td>
</tr>
<tr>
<td>4 f</td>
<td>1/4,3/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 e</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,1/2,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,1/4 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2mm1'
  - \( \mathbf{a}^* = \mathbf{a} \) \( \mathbf{b}^* = \mathbf{b} \)
  - Origin at 0,0,z

- Along [1,0,0] p2mm
  - \( \mathbf{a}^* = \mathbf{b}/2 \) \( \mathbf{b}^* = \mathbf{c}/2 \)
  - Origin at x,0,0

- Along [0,1,0] p2a2mm
  - \( \mathbf{a}^* = \mathbf{c}/2 \) \( \mathbf{b}^* = \mathbf{a}/2 \)
  - Origin at 0,y,1/4
Cccm'  mmm'  Orthorhombic

66.4.567  66.4.567  C2'/c2'/c2/m'

Origin  at center (2/m') at cc2/m'

Asymmetric unit  
0 ≤ x ≤ 1/4;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1 | 0,0,0)

(2)  2  0,0,z
     (2 | 0,0,0)

(3) 2'  0,y,1/4
     (2' | 0,0,1/2)

(4) 2'  x,0,1/4
     (2' | 0,0,1/2)

(5) 1
    (1 | 0,0,0)

(5) m'  x,y,0
     (m' | 0,0,0)

(6) c 0,0,1/2
    (c | 0,0,1/2)

(7) c 0,0,1/2
    (c | 0,0,1/2)

(8) c 0,0,1/2
    (c | 0,0,1/2)

For (1/2,1/2,0) + set

(1) t 1/2,1/2,0
    (1 | 1/2,1/2,0)

(2)  2  1/4,1/4,z
     (2 | 1/2,1/2,0)

(3) 2'  0,1/2,0
     (2' | 1/2,1/2,1/2)

(4) 2'  x,1/4,1/4
     (2' | 1/2,1/2,1/2)

(5) m' 1/4,1/4,0
    (m' | 1/2,1/2,0)

(6) n' 1/2,1/2,0
    (m' | 1/2,1/2,0)

(7) n 1/2,0,1/2
    (m | 1/2,1/2,1/2)

(8) n 0,1/2,1/2
    (m | 1/2,1/2,1/2)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>16 m 1</td>
<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 l .m'</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 k .2</td>
<td>1/4,1/4,z [0,0,w]</td>
<td>3/4,1/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 j .2</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 i .2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 h .2'</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 g .2'</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>4 f .2/m'</td>
<td>1/4,3/4,0 [0,0,0]</td>
<td>3/4,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e .2/m'</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 d .2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2/m'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2'2'</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2'2'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>c2mm</td>
<td>p&lt;sub&gt;2a&lt;/sub&gt;2m'm'</td>
<td>p&lt;sub&gt;2a&lt;/sub&gt;2m'm'</td>
<td></td>
</tr>
<tr>
<td>a* = a  b* = b</td>
<td>a* = -c/2  b* = b/2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,1/4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Note:** The notation and symmetry operations are specific to the crystallographic group Cccm'.
Orthorhombic

Cc'c'm

m'm'm

C2'/c'2'/c'2/m

66.5.568

Origin  at center ( 2/m ) at c'c'2/m

Asymmetric unit

0 ≤ x ≤ 1/4;
0 ≤ y ≤ 1/2;
0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z
(3) 2' 0,y,1/4
(4) 2' x,0,1/4

(1') 0,0,0
(2 z 0,0,0)
(3 y 0,0,1/2)'
(4 x 0,0,1/2)'

(5) 1/4,0,0,0
(6) m x,y,0
(7) c' (0,0,1/2) x,0,z
(8) c' (0,0,1/2) 0,y,z

(1'*) 0,0,0
(2 z* 0,0,0)
(3 y* 0,0,1/2)'
(4 x* 0,0,1/2)'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,2,0)
(2) 2 1/4,1/4,z
(3) 2' (0,1/2,0) 1/4,y,1/4
(4) 2' (1/2,0,0) x,1/4,1/4

(1'*) (1/2,1/2,2,0)
(2 z* 1/2,1/2,2,0)
(3 y* 0,1/2,1/2)'
(4 x* 1/2,1/2,1/2)'

(5) 1/4,1/4,0
(6) n (1/2,1/2,0) x,y,0
(7) n' (1/2,0,1/2) x,1/4,z
(8) n' (0,1/2,1/2) 1/4,y,z

(1'*) 1/4,1/4,0
(2 z* 1/2,1/2,2,0)
(3 y* 0,1/2,1/2)'
(4 x* 1/2,1/2,1/2)'

(5) 1/2,1/2,0
(6) m (1/2,1/2,1/2) x,y,0
(7) m' (1/2,1/2,1/2) x,1/4,z
(8) m' (0,1/2,1/2) 1/4,y,z
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 m</td>
<td>1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>8 l</td>
<td>..m</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>8 k</td>
<td>.2</td>
<td>1/4,1/4,z</td>
</tr>
<tr>
<td>8 j</td>
<td>.2</td>
<td>0,1/2,z</td>
</tr>
<tr>
<td>8 i</td>
<td>.2</td>
<td>0,0,z</td>
</tr>
<tr>
<td>8 h</td>
<td>.2'</td>
<td>0,y,1/4</td>
</tr>
<tr>
<td>8 g</td>
<td>.2'</td>
<td>x,0,1/4</td>
</tr>
<tr>
<td>4 f</td>
<td>.2/m</td>
<td>1/4,3/4,0</td>
</tr>
<tr>
<td>4 e</td>
<td>.2/m</td>
<td>1/4,1/4,0</td>
</tr>
<tr>
<td>4 d</td>
<td>.2/m</td>
<td>0,1/2,0</td>
</tr>
<tr>
<td>4 c</td>
<td>.2/m</td>
<td>0,0,0</td>
</tr>
<tr>
<td>4 b</td>
<td>2'2'</td>
<td>0,1/2,1/4</td>
</tr>
<tr>
<td>4 a</td>
<td>2'2'</td>
<td>0,0,1/4</td>
</tr>
</tbody>
</table>

### Coordinates

- \((x,y,z)\) [u,v,w]
- \((x,y,\bar{z}+1/2)\) [u,v,w]
- \((x,y,z)\) [u,v,w]
- \((x,y,\bar{z}+1/2)\) [u,v,w]

### Symmetry of Special Projections

- Along [0,0,1] c2mm1'
- Along [1,0,0] p2m'm'
- Along [0,1,0] p2mm'

- \(a^* = a\) \(b^* = b\)
- \(a^* = b/2\) \(b^* = c/2\)
- \(a^* = c/2\) \(b^* = a/2\)

Origin at 0,0,z

Origin at x,0,0

Origin at 0,y,0
"Origin at center (2'/m') at cc'2'/m'
Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations
For (0,0,0) + set

(1) 1
(1 | 0,0,0)
(5) 1/4,0,0
(1/2 | 0,0,0)

(2) 2' 0,0,z
(2' | 0,0,0)
(6) m' x,y,0
(m | 0,0,0)

(3) 2' 0,y,1/4
(2' | 0,0,1/2)
(7) c' (0,0,1/2) x,0,z
(c | 0,0,1/2)

(4) 2 x,0,1/4
(2 | 0,0,1/2)
(8) n (0,0,1/2) 0,y,z
(n | 0,0,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,2)
(1/2,1/2,2)
(5) t 1/4,1/4,0
(1/2,1/2,2)

(2) 2' 1/4,1/4,z
(2' | 1/2,1/2,2)
(6) n' (1/2,1/2,2) x,y,0
(n | 1/2,1/2,2)

(3) 2' (0,1/2,0) 1/4,y,1/4
(2' | 1/2,1/2,2)
(7) n' (1/2,0,1/2) x,1/4,z
(n | 1/2,1/2,2)

(4) 2 (1/2,0,0) x,1/4,1/4
(2 | 1/2,1/2,2)
(8) n (0,1/2,1/2) 1/4,y,z
(n | 1/2,1/2,2)

66.6.569 - 1 - 1128
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
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<td>16 m</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 l</td>
<td>x,y,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,y,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 k</td>
<td>1/4,1/4,z [u,v,0]</td>
<td>1/4,3/4,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 j</td>
<td>1/2,1/2,z [u,v,0]</td>
<td>1/2,3/2,z [u,v,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>0,0,z [u,v,0]</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,3/4 [u,0,w]</td>
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<tr>
<td>8 g</td>
<td>x,0,1/4 [u,0,0]</td>
<td>x,0,3/4 [u,0,0]</td>
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<tr>
<td>4 f</td>
<td>1/4,3/4,0 [u,v,0]</td>
<td>3/4,3/4,1/2 [u,v,0]</td>
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<td>4 e</td>
<td>1/4,1/4,0 [u,v,0]</td>
<td>3/4,1/4,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>0,1/2,0 [u,v,0]</td>
<td>0,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>0,0,0 [u,v,0]</td>
<td>0,0,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,1/2,1/4 [u,0,0]</td>
<td>0,1/2,3/4 [u,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,1/4 [u,0,0]</td>
<td>0,0,3/4 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2'mm'</th>
<th>Along [1,0,0]</th>
<th>p2a-2mm</th>
<th>Along [0,1,0]</th>
<th>p2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -c/2</td>
<td>b* = b/2</td>
<td>a* = -a/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (2/m') at c'c'2/m'

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For (0,0,0) + set

1. \((1) \quad (0,0,0)\)
2. \((2) \quad 0,0,z\)
3. \((3) \quad 0,y,1/4\)
4. \((4) \quad x,0,1/4\)
5. \((5) \quad 0,0,0\)
6. \((6) \quad x,y,0\)
7. \((7) \quad c'(0,0,1/2)\)
8. \((8) \quad c'(0,0,1/2)\)

For (1/2,1/2,0) + set

1. \((1) \quad (1/2,1/2,0)\)
2. \((2) \quad 1/4,1/4,z\)
3. \((3) \quad 0,1/2,0\)
4. \((4) \quad x,1/4,1/4\)
5. \((5) \quad 1/4,1/4,0\)
6. \((6) \quad x,y,0\)
7. \((7) \quad n'(1/2,0,1/2)\)
8. \((8) \quad n'(0,1/2,1/2)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>16 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>8 l ..m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 k ..2</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 j ..2</td>
<td>0,1/2,z [0,0,w]</td>
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<tr>
<td>8 i ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 h ..2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 g 2..</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 f ..2/m'</td>
<td>1/4,3/4,0 [0,0,0]</td>
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<tr>
<td>4 e ..2/m'</td>
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<tr>
<td>4 d ..2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c ..2/m'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 222</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 a 222</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2m'm'  
Along [1,0,0] p2m'm'  
Along [0,1,0] p2m'm'

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

\[ a^* = b/2 \quad b^* = c/2 \]

Origin at x,0,0

\[ a^* = c/2 \quad b^* = a/2 \]

Origin at 0,y,0
Origin: at center (2/m) at cc2/m

Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) $T | 0,0,0$
(2) $T | 0,0,z$
(3) $T | y,1/4$
(4) $T | x,0,1/4$

For (1/2,1/2,0)' + set

(5) $T | 1/2,1/2,0$
(6) $T | x,y,0$
(7) $T | 0,0,1/2$
(8) $T | 0,0,1/2$

For (1/2,1/2,0)' + set

(1) $T | 1/2,1/2,0$
(2) $T | 1/4,1/4,z$
(3) $T | 0,1/2,0$
(4) $T | x,1/4,1/4$

(5) $T | 1/2,1/2,0$
(6) $T | x,y,0$
(7) $T | 1/2,1/2,0$
(8) $T | 1/4,1/4,z$

Symmetry Operations

For (0,0,0) + set

(1) $T | 0,0,0$
(2) $T | 0,0,z$
(3) $T | y,1/4$
(4) $T | x,0,1/4$

For (1/2,1/2,0)' + set

(5) $T | 1/2,1/2,0$
(6) $T | x,y,0$
(7) $T | 0,0,1/2$
(8) $T | 0,0,1/2$

For (1/2,1/2,0)' + set

(1) $T' | 1/2,1/2,0$
(2) $T' | 1/4,1/4,z$
(3) $T' | 0,1/2,0$
(4) $T' | x,1/4,1/4$

(5) $T' | 1/2,1/2,0$
(6) $T' | x,y,0$
(7) $T' | 0,0,1/2$
(8) $T' | 0,0,1/2$
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 m 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>8 l ..m</td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td>8 k ..2'</td>
<td>1/4,1/4,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 j ..2</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 i ..2</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 h ..2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 g ..2..</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 f ..2'/m</td>
<td>3/4,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e ..2'/m</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 d ..2/m</td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 c ..2/m</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 b 222</td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 a 222</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] c2mm1'  
  \[a^* = a\quad b^* = b\]
  Origin at 0,0,z

- Along [1,0,0] p2a2m'm'  
  \[a^* = -c/2\quad b^* = b/2\]
  Origin at x,0,0

- Along [0,1,0] p2a2m'm'  
  \[a^* = c/2\quad b^* = a/2\]
  Origin at 0,y,0
Orthorhombic

66.9.572

C<sub>p</sub>\text{c'cm}

mmm1'

C<sub>p</sub>2/c'2'/c2'/m

**Origin** at center (2'/m) at c'c2'/m

**Asymmetric unit**

\[0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

**Symmetry Operations**

For (0,0,0) + set

1. \(1\) \(1 | 0,0,0\)
   \(1 | 0,0,0\)

2. \(2\) \(0,0,z\)
   \(2 | 0,0,0\)'

3. \(3\) \(2\) \(0,y,1/4\)
   \(2 | 0,0,1/2\)'

4. \(4\) \(2\) \(x,0,1/4\)
   \(2 | 0,0,1/2\)

5. \(5\) \(1\) \(0,0,0\)
   \(1 | 0,0,0\)'

6. \(6\) \(m\) \(x,y,0\)
   \(m | 0,0,0\)

7. \(7\) \(c\) \(0,0,1/2\) \(x,0,z\)
   \(m | 0,0,1/2\)

8. \(8\) \(c'\) \(0,0,1/2\) \(0,y,z\)
   \(m | 0,0,1/2\)'

For (1/2,1/2,0) + set

1. \(1\) \(t'\) \(1/2,1/2,0\)
   \(1 | 1/2,1/2,0\)'

2. \(2\) \(2\) \(1/4,1/4,z\)
   \(2 | 1/2,1/2,0\)

3. \(3\) \(2\) \(0,1/2,0\) \(1/4,y,1/4\)
   \(2 | 1/2,1/2,1/2\)

4. \(4\) \(2\) \(1/2,0,0\) \(x,1/4,1/4\)
   \(2 | 1/2,1/2,1/2\)'

5. \(5\) \(1\) \(1/4,1/4,0\)
   \(1 | 1/2,1/2,0\)'

6. \(6\) \(n'\) \(1/2,1/2,0\) \(x,y,0\)
   \(m | 1/2,1/2,0\)'

7. \(7\) \(n'\) \(1/2,1/2,1/2\) \(x,1/4,z\)
   \(m | 1/2,1/2,1/2)'

8. \(8\) \(n\) \(0,1/2,1/2) \(1/4,y,z\)
   \(m | 1/2,1/2,1/2\)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); t’(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0)’ +</td>
</tr>
<tr>
<td>16 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 l ..m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 k ..2</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 j ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 i ..2’</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 h ..2’</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 g ..2</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 f ..2/m’</td>
<td>1/4,3/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 e ..2/m’</td>
<td>1/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 d ..2/m’</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c ..2/m’</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b ..2’</td>
<td>0,1/2,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 a ..2’</td>
<td>0,0,1/4 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2mm1’
- Along [1,0,0] p2mm
- Along [0,1,0] p2a2mm

\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

\[ a^* = b/2 \quad b^* = c/2 \]
Origin at x,0,0

\[ a^* = c/2 \quad b^* = a/2 \]
Origin at 0,y,1/4
Origin at center (2/m') at cc2/m'

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. (1)
   (1|0,0,0)

2. (2) 0, 0, z
   (2|0,0,0)

3. (3) 0, y, 1/4
   (2|0,0,1/2)

4. (4) x, 0, 1/4
   (2|0,0,1/2)

For (1/2,1/2,0) + set

1. (5) 1/4, 1/4, 0
   (1/2,1/2,0)

2. (2) 1/4, 1/4, z
   (1/2,1/2,0)

3. (3) 1/4, y, 1/4
   (1/2,1/2,1/2)

4. (4) x, 1/4, 1/4
   (1/2,1/2,1/2)

For (1/2,1/2,1/2) + set

1. (5) 1/4, 1/4, 0
   (1/2,1/2,0)

2. (2) 1/4, 1/4, z
   (1/2,1/2,0)

3. (3) 1/4, y, 1/4
   (1/2,1/2,1/2)

4. (4) x, 1/4, 1/4
   (1/2,1/2,1/2)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
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</tbody>
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</thead>
<tbody>
<tr>
<td>16 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x',y',z' [u',v',w']</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(8) x,y,z+1/2 [u,v,w]</td>
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<table>
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<tbody>
<tr>
<td>8 l .m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x',y',0 [u',v',0]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
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</thead>
<tbody>
<tr>
<td>8 k .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,z+1/2 [u,v,0]</td>
</tr>
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<td>1/4,3/4,z+1/2 [u,v,0]</td>
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<table>
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<tr>
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<tbody>
<tr>
<td>8 j .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
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<td>0,1/2,z+1/2 [0,0,w]</td>
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<tr>
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<tbody>
<tr>
<td>8 i .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
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<tr>
<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
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</tbody>
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<table>
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<tr>
<th>Positions</th>
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<tbody>
<tr>
<td>8 h .2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g .2'</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
</tr>
</tbody>
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<table>
<thead>
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</tr>
</thead>
<tbody>
<tr>
<td>4 f .2'm'</td>
<td>1/4,3/4,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,1/2 [u,v,0]</td>
</tr>
</tbody>
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<tbody>
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<td>4 e .2'm'</td>
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<td>3/4,1/4,1/2 [u,v,0]</td>
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<tbody>
<tr>
<td>4 d .2'm'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
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<td>0,1/2,1/2 [0,0,0]</td>
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<tbody>
<tr>
<td>4 c .2'm'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
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</thead>
<tbody>
<tr>
<td>4 b 2'2'</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

<table>
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<tr>
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</thead>
<tbody>
<tr>
<td>4 a 2'2'</td>
<td>0,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1] c2mm</th>
<th>Along [1,0,0] p2ac2m'm'</th>
<th>Along [0,1,0] p2ac2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>-a* = -c/2</td>
<td>a* = c/2</td>
<td>a* = c/2</td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = b/2</td>
<td>b* = b/2</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,1/4</td>
<td>Origin at x,0,1/4</td>
<td>Origin at x,0,1/4</td>
</tr>
<tr>
<td>66.10.573 - 2 - 1137</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin: at center (2/m) at c'c'2/m

Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations:

For (0,0,0) + set:

- (1) T 0,0,0
- (2) 2 0,0,z
- (3) 2' 0,y,1/4
- (4) 2' x,0,1/4

For (1/2,1/2,0)' + set:

- (1) T' 1/2,1/2,0)
- (2) 2' 1/4,1/4,z
- (3) 2 (0,1/2,0) 1/4,y,1/4
- (4) 2 (1/2,0,0) x,1/4,1/4

66.11.574 - 1 - 1138
Continued

**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
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<tbody>
<tr>
<td><strong>Along [0,0,1]</strong> c2mm1'</td>
</tr>
<tr>
<td><strong>Along [1,0,0]</strong> p2'mm'</td>
</tr>
<tr>
<td><strong>Along [0,1,0]</strong> p2'mm'</td>
</tr>
<tr>
<td><strong>a</strong> = a <strong>b</strong> = b</td>
</tr>
<tr>
<td><strong>a</strong> = -c/2 <strong>b</strong> = b/2</td>
</tr>
<tr>
<td><strong>a</strong> = c/2 <strong>b</strong> = a/2</td>
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</tbody>
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<table>
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<tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
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<tr>
<td>(1/2,1/2,0)' +</td>
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<td><strong>Multiplicity, Wyckoff letter, Site Symmetry.</strong></td>
</tr>
<tr>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>16 m 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) x,y,z [u,v,w] (8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 l ..m x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 k ..2' 1/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>8 j ..2 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 i ..2 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 h ..2' 0,y,1/4 [u,0,w] 0,y,1/4 [u,0,w] 0,y,1/4 [u,0,w] 0,y,1/4 [u,0,w] 0,y,1/4 [u,0,w] 0,y,1/4 [u,0,w] 0,y,1/4 [u,0,w] 0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 g ..2' x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>4 f ..2'm 1/4,3/4,0 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e ..2'm 1/4,1/4,0 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 d ..2'm 0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c ..2'm 0,0,0 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2'2' 0,1/2,1/4 [0,0,0] 0,1/2,3/4 [0,0,0] 0,1/2,3/4 [0,0,0] 0,1/2,3/4 [0,0,0] 0,1/2,3/4 [0,0,0] 0,1/2,3/4 [0,0,0] 0,1/2,3/4 [0,0,0] 0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2'2' 0,0,1/4 [0,0,0] 0,0,3/4 [0,0,0] 0,0,3/4 [0,0,0] 0,0,3/4 [0,0,0] 0,0,3/4 [0,0,0] 0,0,3/4 [0,0,0] 0,0,3/4 [0,0,0] 0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>
**Origin** at center (2/m') at cc'2'/m'

**Asymmetric unit**  \(0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

**Symmetry Operations**

For (0,0,0) + set

1. \(I \quad (0,0,0)\)
2. \(2' \quad 0,0,z\) \( (2_z,0,0)' \)
3. \(2' \quad 0,y,1/4\) \( (2_z,0,0.1/2)' \)
4. \(2 \quad x,0,1/4\) \( (2_x,0,0.1/2) \)
5. \( m' \quad x,y,0\) \( (m_z,0,0,0)' \)
6. \( c' \quad (0,0,1/2)\) \( x,0,z\) \( (m_y,0,0.1/2)' \)
7. \( c \quad (0,0,1/2)\) \( 0,y,z\) \( (m_z,0,0.1/2) \)

For (1/2,1/2,0) + set

1. \(t' \quad (1/2,1/2,2,0)\) \( (1,1/2,1/2,2,0)' \)
2. \(2 \quad 1/4,1/4,z\) \( (2_z,1/2,1/2,2,0) \)
3. \(2 \quad (0,1/2,0)\) \( 1/4,y,1/4\) \( (2_y,1/2,1/2,2,0)' \)
4. \(2' \quad (1/2,0,0)\) \( x,1/4,1/4\) \( (2_x,1/2,1/2,2,0)' \)
5. \( n' \quad 1/4,1/4,0\) \( (1/2,1/2,2,0)' \)
6. \(n \quad (1/2,1/2,2,0)\) \( x,y,0\) \( (m_z,1/2,1/2,2,0) \)
7. \(n \quad (1/2,0,1/2)\) \( x,1/4,z\) \( (m_y,1/2,1/2,2,0)' \)
8. \(n \quad (1/2,1/2,2,0)' \) \( 1/4,y,z\) \( (m_z,1/2,1/2,2,0)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) x,y,z+1/2 [u,v,w]</td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(6)</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td>(7) x,y,z+1/2 [u,v,w]</td>
<td>(8) x,y,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c22mm'  Along [1,0,0] p2a2mm  Along [0,1,0] p222m

a* = a  b* = b  a* = -a/2  b* = b/2  a* = -a/2  b* = c/2

Origin at 0,0,z  Origin at 0,0,0  Origin at 0,y,0
**Origin** at center (2/m) at c'c'2/m'

**Asymmetric unit**

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For $$(0,0,0)$$ + set

1. $$(1) \quad 0,0,0$$
   
2. $$(2) \quad 2 \cdot 0,0,z$$
   
3. $$(3) \quad 2 \cdot 0,0,1/2$$

For $$(1/2,1/2,0)'$$ + set

1. $$(1) \quad t' (1/2,1/2,0)$$

2. $$(2) \quad 2' \cdot 1/4,1/4,z$$

3. $$(3) \quad 2' (0,1/2,0) \cdot 1/4,y,1/4$$

4. $$(4) \quad 2' (1/2,0,0) \cdot 1/4,1/4$$

5. $$(5) \quad 1/4,1/4,0$$

6. $$(6) \quad n (1/2,1/2,0) \cdot x,y,0$$

7. $$(7) \quad n (1/2,0,1/2) \cdot x,1/4,z$$

8. $$(8) \quad n (0,1/2,1/2) \cdot 1/4,y,z$$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>16 m</td>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>8 l ..m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 k ..2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td>8 j ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 i ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 h ..2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 g ..1</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 f ..2'/m'</td>
<td>1/4,3/4,0 [u,v,0]</td>
</tr>
<tr>
<td>4 e ..2'/m'</td>
<td>1/4,1/4,0 [u,v,0]</td>
</tr>
<tr>
<td>4 d ..2/m'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c ..2/m'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 222</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 a 222</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2m'm'  Along [1,0,0] p2m'm'  Along [0,1,0] p2m'm'
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
\( \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)
\( \mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = \mathbf{a}/2 \)

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Origin  at center (2/m) at 2/m21/aa

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1) 0,0,0
   (2) 1/4,0,z
   (2) 1/2,0,0
   (3) 1/4,y,0
   (3) 1/2,0,0
   (4) 2 x,0,0
   (2) 0,0,0

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
   (1) 1/2,1/2,0
   (2) 0,1/4,z
   (2) 0,1/2,0
   (3) 0,1/2,0
   (3) 0,1/2,0
   (4) 2 (1/2,0,0) x,1/4,0
   (2) 1/2,1/2,0

(5) 1/4,1/4,0
   (1) 1/2,1/2,0
   (6) b (0,1/2,0)
   (6) 0,1/2,0
   (7) m x,1/4,z
   (7) m,0,1/2,0
   (8) b (0,1/2,0) 1/4,y,z
   (8) m,1/2,1/2,0

Cmma  mmm  Orthorhombic

67.1.577  C2/m2/m2/a
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2, y+z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u,v,w]</td>
<td>(3) x+1/2, y, z [u,v,w]</td>
</tr>
<tr>
<td>8 n.m.</td>
<td>x,1/4, z [0,v,0]</td>
<td>x,3/4, z [0,v,0]</td>
</tr>
<tr>
<td>8 m m..</td>
<td>0,y,z [0,0,0]</td>
<td>0,y+1/2, z [u,0,0]</td>
</tr>
<tr>
<td>8 l ..2</td>
<td>1/4,0, z [0,0,w]</td>
<td>3/4,1/2, z [0,0,w]</td>
</tr>
<tr>
<td>8 k ..2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
<td>3/4,y +1/2, 1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 j ..2.</td>
<td>1/4,y,0 [0,v,0]</td>
<td>3/4,y +1/2, 0 [0,v,0]</td>
</tr>
<tr>
<td>8 i ..2.</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 h ..2.</td>
<td>x,0,0 [u,0,0]</td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 g mm2</td>
<td>0,1/4, z [0,0,0]</td>
<td>0,3/4, z [0,0,0]</td>
</tr>
<tr>
<td>4 f .2/m.</td>
<td>1/4,1/4,1/2 [0,v,0]</td>
<td>3/4,1/4,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 e .2/m.</td>
<td>1/4,1/4,0 [0,v,0]</td>
<td>3/4,1/4,0 [0,v,0]</td>
</tr>
<tr>
<td>4 d 2/m..</td>
<td>0,0,1/2 [u,0,0]</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 c 2/m..</td>
<td>0,0,0 [u,0,0]</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 b 222</td>
<td>1/4,0,1/2 [0,0,0]</td>
<td>3/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 222</td>
<td>1/4,0,0 [0,0,0]</td>
<td>3/4,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_c 2mm  
\(a^* = a/2\) \(b^* = b/2\)  
Origin at 0,1/4,z

Along [1,0,0] p2mm 1'  
\(a^* = b/2\) \(b^* = c\)  
Origin at x,0,0

Along [0,1,0] p_{2a} 2m'  
\(a^* = c\) \(b^* = a/2\)  
Origin at 1/4,y,0

67.1.577 - 2 - 1145
Cmma1

Orthorhombic

67.2.578

C2/m2/m2/a1

Origin at center (2/m1') at 2/m2/aa1'

Asymmetric unit

0 < x < 1/2; 0 < y < 1/4; 0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

(1) t (1 | 0,0,0)
(2) 2 1/4,0,z
(3) 2 1/4,y,0 (4) 2 x,0,0
(5) 2 1/2,0,0
(6) a (1/2,0,0) x,y,0 (7) a (1/2,0,0) x,0,z
(8) m 0,y,z
(1*) 1/2,0,0
(2 z* 1/2,0,0)
(2 y* 1/2,0,0)
(2 x* 0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1) 1/2,1/2,0)
(2) 2 0,1/4,z (3) 2 (0,1/2,0) 0,y,0 (4) 2 (1/2,0,0) x,1/4,0
(5) 2 0,1,2,0)
(2 z* 0,1,2,0)
(2 y* 0,1,2,0)
(2 x* 1/2,1/2,0)

For (0,0,0)' + set

(1) t (1' | 0,0,0)' (1* 0,0,0)'
(2) 2' 1/4,0,z
(3) 2' 1/4,y,0 (4) 2' x,0,0
(5) 2' 1/2,0,0' (6) a' (1/2,0,0) x,y,0
(7) a' (1/2,0,0) x,0,z
(8) m' 0,y,z
(1* 0,0,0)'
(2 z* 1/2,0,0)'
(2 y* 1/2,0,0)'
(2 x* 1/2,1/2,0)'

For (1/2,1/2,0)'+ set

(1) t (1'/2,1/2,0)'
(1' 1/2,1/2,0)'
(2) 2' 0,1/4,z
(3) 2' (0,1/2,0) 0,y,0 (4) 2' (1/2,0,0) x,1/4,0
(5) 2' 1/2,0,0' (6) b' (0,1/2,0) x,y,0
(7) m' x,1/4,z (8) b' (0,1/2,0) 1/4,y,z
(1* 1/2,1/2,0)'
(2 z* 1/2,0,0)'
(2 y* 1/2,0,0)'
(2 x* 1/2,1/2,0)'

67.2.578 - 1 - 1146
Generators selected: \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5); 1'\).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 o 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) (x+1/2,y,z) [0,0,0]</td>
</tr>
<tr>
<td>8 n .m. 1'</td>
<td>x,1/4,z [0,0,0]</td>
<td>x,1/4,z [0,0,0]</td>
</tr>
<tr>
<td>8 m m.. 1'</td>
<td>0,y,z [0,0,0]</td>
<td>0,y+1/2,z [0,0,0]</td>
</tr>
<tr>
<td>8 l ..21'</td>
<td>1/4,0,z [0,0,0]</td>
<td>3/4,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>8 k .2.1'</td>
<td>1/4,y,1/4 [0,0,0]</td>
<td>3/4,y+1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 j .2.1'</td>
<td>1/4,y,0 [0,0,0]</td>
<td>3/4,y+1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>8 i 2..1'</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 h 2..1'</td>
<td>x,0,0 [0,0,0]</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 g mm21'</td>
<td>0,1/4,z [0,0,0]</td>
<td>0,3/4,z [0,0,0]</td>
</tr>
<tr>
<td>4 f .2/m.1'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e .2/m.1'</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>4 d 2/m..1'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c 2/m..1'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2221'</td>
<td>1/4,0,1/2 [0,0,0]</td>
<td>3/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2221'</td>
<td>1/4,0,0 [0,0,0]</td>
<td>3/4,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1] p2mm1'  
\(a^* = a/2\)  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\(a^* = b/2\)  
Origin at x,0,0

Along [0,1,0] p2mm1'  
\(a^* = c\)  
Origin at y,0,0
Cm'ma  
67.3.579

m'mm  
C2/m'2'/m2'/a

Orthorhombic

Origin  at center (2/m') at 2/m'2', 'aa

Asymmetric unit  
0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/4;  0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2' 1/4,0,z
(2z | 1/2,0,0)'

(5) 1'
(0,0,0)'

(6) a (1/2,0,0) x,y,0
(mz | 1/2,0,0)

(10) a (1/2,0,0) x,0,z
(2y | 1/2,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,2,0)
(1 | 1/2,1/2,0)

(2) 2' 0,1/4,z
(2z | 0,1/2,0)'

(5) 1'
(1/2,1/2,0)'

(6) b (0,1/2,0) x,y,0
(mz | 0,1/2,0)

(10) m x,1/4,z
(2y | 0,1/2,0)

(8) b' (0,1/2,0) 1/4,y,z
(mz | 1/2,1/2,0)'

67.3.579 - 1 - 1148
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w] (2) x +1/2, y, z [u,v,w] (3) x +1/2, y, z [u,v,w] (4) x, y, z [u,v,w] (5) x, y, z [u,v,w] (6) x +1/2, y, z [u,v,w] (7) x +1/2, y, z [u,v,w] (8) x, y, z [u,v,w]</td>
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<td>x,1/4, z [0,v,0] x,3/4, z [0,v,0] x,3/4, z [0,v,0]</td>
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<tr>
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<tr>
<td>8 i 2.. 8</td>
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<tr>
<td>4 f .2'/m. 4</td>
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<tr>
<td>4 e .2'/m. 4</td>
<td>1/4,1/4,0 [0,0,0] 3/4,1/4,0 [0,0,0]</td>
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<tr>
<td>4 d 2/m'.. 4</td>
<td>0,0,1/2 [0,0,0] 0,1/2,1/2 [0,0,0]</td>
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<tr>
<td>4 c 2/m'.. 4</td>
<td>0,0,0 [0,0,0] 0,1/2,0 [0,0,0]</td>
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<tr>
<td>4 b 22'2' 4</td>
<td>1/4,0,1/2 [u,0,0] 3/4,0,1/2 [u,0,0]</td>
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<td>4 a 22'2' 4</td>
<td>1/4,0,0 [u,0,0] 3/4,0,0 [u,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p_{c-}2mm Along [1,0,0] p2mm Along [0,1,0] p_{2a}.2m'm'
a* = a/2 b* = b/2 a* = b/2 b* = c a* = -a/2 b* = c
Origin at 1/4,1/4,z Origin at x,0,0 Origin at 0,y,0
**Symmetry Operations**

For (0,0,0) + set

1. \( I \) \((0,0,0)\)
2. \( 2 \) 1/4,0,z
   \((2_z|1/2,0,0)\)
3. \( 2' \) 1/4,y,0
   \((2_z|1/2,0,0)'\)
4. \( 2' \) x,0,0
   \((2_z|0,0,0)'\)

5. \( T \) 0,0,0
   \((1/2,0,0)'\)
6. \( a' \) (1/2,0,0) x,y,0
   \((m_z|1/2,0,0)'\)
7. \( a \) (1/2,0,0) x,0,z
   \((m_y|1/2,0,0)\)
8. \( m \) 0,y,z
   \((m_z|0,0,0)\)

For (1/2,1/2,0) + set

1. \( t \) (1/2,1/2,0)
   \((1|1/2,1/2,0)\)
2. \( 2 \) 0,1/4,z
   \((2_z|0,1/2,0)\)
3. \( 2' \) (0,1/2,0) 0,y,0
   \((2_y|0,1/2,0)'\)
4. \( 2' \) (1/2,0,0) x,1/4,0
   \((2_z|1/2,1/2,0)'\)

5. \( T \) 1/4,1/4,0
   \((1/2,1/2,0)'\)
6. \( b' \) (0,1/2,0) x,y,0
   \((m_z|0,1/2,0)'\)
7. \( m \) x,1/4,z
   \((m_y|0,1/2,0)\)
8. \( b \) (0,1/2,0) 1/4,y,z
   \((m_z|1/2,1/2,0)\)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

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<td>(1) x,y,z [u,v,w]</td>
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<td>(5) x ,y ,z [ū,v,w]</td>
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<td>8 n</td>
<td>x,1/4,z [0,v,0]</td>
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<tr>
<td>8 m</td>
<td>0,y,z [u,0,0]</td>
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<tr>
<td>8 l</td>
<td>1/4,0,z [0,0,w]</td>
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<tr>
<td>8 k</td>
<td>1/4,y,1/4 [u,0,w]</td>
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<tr>
<td>8 j</td>
<td>1/4,y,0 [u,0,w]</td>
</tr>
<tr>
<td>8 i</td>
<td>x,0,1/2 [0,v,w]</td>
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<tr>
<td>8 h</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
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<td>0,1/4,z [0,0,0]</td>
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<tr>
<td>4 f</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
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<td>4 e</td>
<td>1/4,1/4,0 [0,0,0]</td>
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<td>4 d</td>
<td>0,0,1/2 [0,0,0]</td>
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<td>4 c</td>
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<td>1/4,0,0 [0,0,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2mm

\[ a^* = a/2 \quad b^* = b/2 \]

Origin at 0,0,z

Along [1,0,0] p2mm1'

\[ a^* = b/2 \quad b^* = c \]

Origin at 0,0,0

Along [0,1,0] p2a2mm

\[ a^* = -a/2 \quad b^* = c \]

Origin at 0,y,0
Origin: at center (2'/m') at 2'/m'2'/a'

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) t (0,0,0)
   (1|0,0,0)
   (1|0,0,0)
(2) 2 1/4,0,z
   (2z|1/2,0,0)
   (5) 1/4,0,0
   (0,0,0)
   (5|0,0,0)
   (5|0,0,0)
(6) a (1/2,0,0)
   (mz|1/2,0,0)
   (7) a' (1/2,0,0)
   (mx|1/2,0,0)
   (8) m' 0,y,z
   (mz|0,0,0)
   (mz|0,0,0)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
   (1|1/2,1/2,0)
   (5|1/2,1/2,0)
(2) 2 0,1/4,z
   (2z|0,1/2,0)
   (6) b (0,1/2,0)
   (mz|0,1/2,0)
   (7) m' x,1/4,z
   (mz|0,1/2,0)
   (8) b' (0,1/2,0) 1/4,y,z
   (mz|1/2,1/2,0)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
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<td>(0,0,0)</td>
<td>(1,1/2,1/2,0)</td>
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<td>16 o 1</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td>(5) -</td>
<td>x,y,z [u,v,w]</td>
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</tr>
<tr>
<td>8 n .m.'</td>
<td>x/1/4,z [u,0,w]</td>
<td></td>
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<tr>
<td>(6) -</td>
<td>x/1/4,z [u,0,w]</td>
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</tr>
<tr>
<td>8 m m'</td>
<td>0,y,z [0,v,w]</td>
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<tr>
<td>(7) -</td>
<td>0,y+1/2,z [0,v,w]</td>
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<td>1/4,0,z [0,0,w]</td>
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<td>(8) -</td>
<td>1/4,0,z [0,0,w]</td>
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<tr>
<td>8 k .2'</td>
<td>1/4,y,1/4 [u,0,w]</td>
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<td>(9) -</td>
<td>1/4,y,1/4 [u,0,w]</td>
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<tr>
<td>8 j .2'</td>
<td>1/4,y,0 [u,0,w]</td>
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<td>(10) -</td>
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<td>8 i .2'</td>
<td>x,0,1/2 [0,v,w]</td>
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<td>4 g m'm'2</td>
<td>0,1/4,z [0,0,w]</td>
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<td>(13) -</td>
<td>0,1/4,z [0,0,w]</td>
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<tr>
<td>4 f .2'/m'</td>
<td>1/4,1/4,1/2 [u,0,w]</td>
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<td>(14) -</td>
<td>1/4,1/4,1/2 [u,0,w]</td>
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<td>4 e .2'/m'</td>
<td>1/4,1/4,0 [u,0,w]</td>
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<td>(15) -</td>
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<td>4 d 2'/m'..</td>
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<td>(16) -</td>
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<td>4 c 2'/m'..</td>
<td>0,0,0 [0,v,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p_c-2mm  
Along [0,1,0] p2'mm'  
Along [0,1,0] p2'mm'  

\[ a^* = a/2 \quad b^* = b/2 \]
\[ a^* = c \quad b^* = b/2 \]
\[ a^* = c \quad b^* = a/2 \]

Origin at 1/4,0,0
Origin at x,0,0
Origin at 0,y,0
Cm'm'α'  
67.6.582  
mm'm'  
C2/m2'/m2'/α'

**Origin**  at center (2/m) at 2/m2'/a'a'

**Asymmetric unit**  
0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/4;  0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

1. $t(0,0,0)$
2. $t(1/2,0,0)'
3. $t(1/2,1/2,0)$
4. $t(1/2,1/2,0)'$

For (1/2,1/2,0) + set

1. $t(1/2,0,0)$
2. $t(0,1/2,0)'
3. $t(0,1/2,0)$
4. $t(1/2,0,0)'$

6. $a'(1/2,0,0) x,y,0$
7. $a'(1/2,0,0) x,0,z$
8. $m 0,y,z$
9. $m 0,0,0$

10. $b'(0,1/2,0) x,y,0$
11. $m x,1/4,z$
12. $b (0,1/2,0) 1/4,y,z$
13. $m 1/2,1/2,0$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(1) x,y,z [u,v,w]</td>
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<td>(6) x +1/2,y,z [u,v,w]</td>
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<td>x,1/4,z [u,0,w]</td>
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<td>0,y,z [u,0,0]</td>
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<td>8 l .2'</td>
<td>1/4,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 k .2'</td>
<td>1/4,y,1/4 [u,0,w]</td>
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<td>8 j .2'</td>
<td>1/4,y,0 [u,0,w]</td>
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<td>x,0,1/2 [u,0,0]</td>
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<td>x,0,0 [u,0,0]</td>
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<td>4 g mm'2'</td>
<td>0,1/4,z [u,0,0]</td>
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<td>4 f .2'm'</td>
<td>1/4,1/4,1/2 [u,0,w]</td>
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<td>4 e .2'm'</td>
<td>1/4,1/4,0 [u,0,w]</td>
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<td>4 d 2/m.</td>
<td>0,0,1/2 [u,0,0]</td>
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<td>4 c 2/m.</td>
<td>0,0,0 [u,0,0]</td>
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<tr>
<td>4 a 22'2</td>
<td>1/4,0,0 [u,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2'mm'  
Along [1,0,0] p2mm1'  
Along [0,1,0] p2'mm'  
a* = a/2  
b* = b/2  
a* = a/2  
b* = c  
Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at center (2/m') at 2/m'2/a'a'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. t (x,0,0)
   1' (1/2,0,0)

2. 2 1/4,0,z
   2' 1/2,0,0

3. 2 1/4,y,0
   2' 1/2,0,0

4. 2 x,0,0
   2' 0,0,0

5. t - 0,0,0
   1/2,0,0

6. a' (1/2,0,0)
   m'_1/2,0,0

7. a' (1/2,0,0)
   m'_1/2,0,0

8. m' 0,y,z
   m'_0,0,0

For (1/2,1/2,0) + set

1. t (1/2,1/2,0)
   1' 1/2,1/2,0

2. 2 0,1/4,z
   2' 0,1/2,0

3. 2 (0,1/2,0) 0,y,0
   2' 0,1/2,0

4. 2 (1/2,0,0) x,1/4,0
   2' 1/2,1/2,0

5. t - 1/4,1/4,0
   1/2,1/2,0

6. b' (0,1/2,0) x,y,0
   m'_0,1/2,0

7. m' x,1/4,z
   m'_0,1/2,0

8. b' (0,1/2,0) 1/4,y,z
   m'_1/2,1/2,0
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

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<td>(2) x+1/2, y, z [u, v, w]</td>
<td>(0,0,0) +</td>
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<td>(3) x+1/2, y, z [u, v, w]</td>
<td>(1/2,1/2,0) +</td>
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<td>(5) x, y, z [u, v, w]</td>
<td>(6) x+1/2, y, z [u, v, w]</td>
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<tr>
<td>8 n .m'</td>
<td>x,1/4, z [u,0,w]</td>
<td>x,1/4, z [u,0,w]</td>
<td>x,1/4, z [u,0,w]</td>
</tr>
<tr>
<td>8 m m'</td>
<td>0,y,z [0,v,w]</td>
<td>0,y+1/2,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 l ..2</td>
<td>1/4,0,z [0,0,w]</td>
<td>1/4,1/2,z [0,0,w]</td>
<td>1/4,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 k .2</td>
<td>1/4,y,1/4 [0,v,0]</td>
<td>1/4,y+1/2,1/2 [0,v,0]</td>
<td>1/4,y+1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 j .2</td>
<td>1/4,y,0 [0,v,0]</td>
<td>1/4,y+1/2,0 [0,v,0]</td>
<td>1/4,y+1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>8 i 2..</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 h 2..</td>
<td>x,0,0 [u,0,0]</td>
<td>x,1/2,0 [u,0,0]</td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 g m'm'2</td>
<td>0,1/4,z [0,0,w]</td>
<td>0,3/4,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 f .2/m'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e .2/m'</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 d .m'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 c 2/m'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b 222</td>
<td>1/4,0,1/2 [0,0,0]</td>
<td>3/4,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a 222</td>
<td>1/4,0,0 [0,0,0]</td>
<td>3/4,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2m'm'  
  a*=a/2  b*=b/2  Origin at 0,0,z

- Along [1,0,0] p2m'm'  
  a*=b/2  b*=c  Origin at x,0,0

- Along [0,1,0] p2m'm'  
  a*=c  b*=a/2  Origin at 0,y,0
**C2c mma**

67.8.584

**Orthorhombic**

C2c 2/m2/m2/a

**Asymmetric unit**

\[0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{4}; \quad 0 < z < \frac{1}{2}\]

**Symmetry Operations**

For \(0,0,0\) + set

1. \(I \quad (0,0,0)\)
2. \(\bar{1} \quad \frac{1}{2},0,0\)
3. \(a \quad \frac{1}{2},0,0\)
4. \(b \quad 0,0,0\)
5. \(c \quad 0,0,1\)
6. \(d \quad 0,1,0\)
7. \(e \quad 1,0,0\)
8. \(f \quad 0,0,1\)

For \(1/2,1/2,0\) + set

1. \(t \quad \frac{1}{2},1/2,0\)
2. \(\bar{t} \quad 0,1/2,0\)
3. \(a' \quad 1/2,0,1\)
4. \(b' \quad 0,1/2,1\)
5. \(c' \quad 1/2,1/2,1\)
6. \(d' \quad 0,1/2,1\)
7. \(e' \quad 1/2,0,1\)
8. \(f' \quad 0,0,1\)

For \(0,0,1\) + set

1. \(t' \quad \frac{1}{2},1/2,1\)
2. \(\bar{t}' \quad 0,1/2,1\)
3. \(a'' \quad 1/2,0,1\)
4. \(b'' \quad 0,1/2,1\)
5. \(c'' \quad 1/2,1/2,1\)
6. \(d'' \quad 0,1/2,1\)
7. \(e'' \quad 1/2,0,1\)
8. \(f'' \quad 0,0,1\)

For \(1/2,1/2,1\) + set

1. \(t'' \quad \frac{1}{2},1/2,1\)
2. \(\bar{t}'' \quad 0,1/2,1\)
3. \(a''' \quad 1/2,0,1\)
4. \(b''' \quad 0,1/2,1\)
5. \(c''' \quad 1/2,1/2,1\)
6. \(d''' \quad 0,1/2,1\)
7. \(e''' \quad 1/2,0,1\)
8. \(f''' \quad 0,0,1\)
Generators selected: (1); t(1,0,0); t(0,1,0); t'(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z [u,v,w]</td>
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<tr>
<td>16 n .m.</td>
<td>x,1/4,z [u,v,0]</td>
<td>x,1/4,z [u,v,0]</td>
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<tr>
<td>16 m ..</td>
<td>0,y,z [u,0,0]</td>
<td>0,y+1/2,z [u,0,0]</td>
</tr>
<tr>
<td>16 l ..2</td>
<td>1/4,0,z [0,0,w]</td>
<td>3/4,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>16 k ..2'</td>
<td>1/4,y,1/4 [u,0,w]</td>
<td>3/4,y+1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>16 j ..2</td>
<td>1/4,y,0 [u,0,v]</td>
<td>3/4,y+1/2,0 [u,0,v]</td>
</tr>
<tr>
<td>16 i ..2'</td>
<td>x,0,1/2 [v,0,w]</td>
<td>x,0,1/2 [v,0,w]</td>
</tr>
<tr>
<td>16 h ..2</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>8 g mm2</td>
<td>0,1/4,z [0,0,0]</td>
<td>0,3/4,z [0,0,0]</td>
</tr>
<tr>
<td>8 f .2/m.</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 e .2/m.</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>8 d .2/m.</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 c .2/m.</td>
<td>0,0,0 [u,0,0]</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>8 b 2'2</td>
<td>1/4,0,1/2 [0,0,w]</td>
<td>3/4,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 a 222</td>
<td>1/4,0,0 [0,0,0]</td>
<td>3/4,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm1'
  \[a^* = a/2 \quad b^* = b/2\]
  Origin at 0,0,z

- Along [1,0,0] p2mm1'
  \[a^* = b/2 \quad b^* = c\]
  Origin at x,0,0

- Along [0,1,0] p2mm1'
  \[a^* = c \quad b^* = a/2\]
  Origin at 1/2,y,0

67.8.584 - 2 - 1159
Origin at center (2/m) at 2/m2/1/aa

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) \( T_1 \)
(1 | 0,0,0)

(2) \( 2_{1} \) 1/4,0,z
(2_1 | 1/2,0,0)

(3) \( 2_{1} \) 1/4,y,0
(2_1 | 1/2,0,0)

(4) \( 2_{1} \) x,0,0
(2_1 | 0,0,0)

(5) \( T_1 \)
(1 | 0,0,0)

(6) a (1/2,0,0) x,y,0
(m_1 | 1/2,0,0)

(7) a (1/2,0,0) x,0,z
(m_1 | 1/2,0,0)

(8) m 0,y,z
(m_1 | 0,0,0)

For (1/2,1/2,0)' + set

(1) \( T_1 \)
(1 | 1/2,1/2,0)

(2) \( 2' \) 0,1/4,z
(2_1 | 0,1/2,0)

(3) \( 2' \) (0,1/2,0) 0,y,0
(2_1 | 0,1/2,0)

(4) \( 2' \) (1/2,0,0) x,1/4,0
(2_1 | 1/2,0,0)

(5) \( T_1 \)
(1 | 1/2,1/2,0)

(6) b' (0,1/2,0) x,y,0
(m_1 | 0,1/2,0)

(7) m' x,1/4,z
(m_1 | 0,1/2,0)

(8) b' (0,1/2,0) 1/4,y,z
(m_1 | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry. Coordinates

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 o 1</td>
<td>16</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>8 n .m'</td>
<td>8</td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td>8 m m..</td>
<td>8</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>8 l .2</td>
<td>8</td>
<td>1/4,0,0</td>
</tr>
<tr>
<td>8 k .2</td>
<td>8</td>
<td>1/4,0,0</td>
</tr>
<tr>
<td>8 j .2</td>
<td>8</td>
<td>1/4,0,0</td>
</tr>
<tr>
<td>8 i .2</td>
<td>8</td>
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<tr>
<td>8 h .2</td>
<td>8</td>
<td>1/4,0,0</td>
</tr>
<tr>
<td>4 g m'm'2</td>
<td>4</td>
<td>0,1/4,0</td>
</tr>
<tr>
<td>4 f .2/m'</td>
<td>4</td>
<td>1/4,1/4,1/2</td>
</tr>
<tr>
<td>4 e .2/m'</td>
<td>4</td>
<td>1/4,1/4,1/2</td>
</tr>
<tr>
<td>4 d 2/m..</td>
<td>4</td>
<td>0,1/2,1/2</td>
</tr>
<tr>
<td>4 c 2/m..</td>
<td>4</td>
<td>0,1/2,1/2</td>
</tr>
<tr>
<td>4 b 222</td>
<td>4</td>
<td>1/4,0,0</td>
</tr>
<tr>
<td>4 a 222</td>
<td>4</td>
<td>3/4,0,0</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  \( p_{2a}.2m'1' \)  \( a^* = a/2 \)  \( b^* = b/2 \)  Origin at 1/4,0,z
Along [1,0,0]  \( p2mm1' \)  \( a^* = b/2 \)  \( b^* = c \)  Origin at x,0,0
Along [0,1,0]  \( p_{2a}.2m'1' \)  \( a^* = -a/2 \)  \( b^* = c \)  Origin at 1/4,y,0

C_{pmmma}
C1, mma
67.10.586
Orthorhombic

mmm1’
C1, 2/m2/m2/a

Origin at center (2/m) at 2/m2/m/a

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. (1,0,0,0)
2. (2, 1/4,0,z)
3. (3, 1/4,y,0)
4. (4, x,0,0)

For (1/2,1/2,0)’ + set

(1) t’ (1/2,1/2,0)
(1) 1/2,1/2,0)
(2) 2’ (0,1/4,z)
(2) 1/2,0,0)
(3) 2’ (0,1/2,0) 0,y,0
(3) 0,0,1/2
(4) 2’ (1/2,0,0) x,1/4,0
(4) 2,0,0

For (0,0,1)’ + set

(1) t’ (0,0,1)
(1) 0,0,1)
(2) 2’ (0,0,1) 1/4,0,z
(2) 1/2,0,1)
(3) 2’ (0,0,1) 1/4,y,1/2
(3) 0,1/2,0)
(4) 2’ x,0,1/2
(4) 2,1/2,0)

For (1/2,1/2,1) + set

(1) t (1/2,1/2,1)
(1) 1/2,1/2,1)
(2) 2 (0,0,1) 0,1/4,z
(2) 0,1/2,1)
(3) 2 (0,1/2,0) 0,y,1/2
(3) 0,1/2,1)
(4) 2 (1/2,0,0) x,1/4,1/2
(4) 0,1/2,1)

For (1/4,1/4,1/2) + set

(1) t (1/4,1/4,1/2)
(1) 1/4,1/4,1/2)
(2) 2 (0,1/2,0) x,y,1/2
(2) 0,1/2,1)
(3) 2 (0,0,1) x,1/4,z
(3) 0,1/2,1)
(4) 2 (1/2,0,0) x,1/4,1/2
(4) 0,1/2,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
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</tr>
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<tbody>
<tr>
<td>32 o 1</td>
<td>(0,0,0) + (1/2,1/2,0)</td>
</tr>
<tr>
<td>(0,0,1)' +</td>
<td>(1/2,1/2,1)</td>
</tr>
<tr>
<td>(5) x, y, z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(6) x, y, z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(7) x, y, z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(8) x, y, z</td>
<td>[u,v,w]</td>
</tr>
</tbody>
</table>

| 16 n.m'  | x,1/4,z [u,0,w] |
| 16 m..  | 0,y,z [u,0,0] |
| 16 l..  | 1/4,0,z [0,0,w] |
| 16 k..  | 1/4,y,1/4 [u,0,w] |
| 16 j..  | 1/4,y,0 [0,0,0] |
| 16 i..  | x,0,1/2 [0,v,w] |
| 16 h..  | x,0,0 [u,0,0] |
| 8 g m'm' | 0,1/4,z [0,0,w] |
| 8 f m'.. | 1/4,1/4,1/2 [u,0,w] |
| 8 e m'.. | 1/4,1/4,0 [0,0,0] |
| 8 d m..  | 0,0,1/2 [0,0,0] |
| 8 c m..  | 0,0,0 [u,0,0] |
| 8 b c'2  | 1/4,0,1/2 [0,0,w] |
| 8 a 222  | 1/4,0,0 [0,0,0] |

**Symmetry of Special Projections**

- Along [0,0,1] p2mm1'
  - $a^* = a/2$  
  - $b^* = b/2$
  - Origin at 0,0,z

- Along [1,0,0] p2mm1'
  - $a^* = b/2$  
  - $b^* = c$
  - Origin at x,0,0

- Along [0,1,0] p2mm1'
  - $a^* = c$  
  - $b^* = a/2$
  - Origin at 1/2,y,0
### Symmetry Operations

#### For (0,0,0) + set

1. $1$
2. $2'$ 1/4,0,z
3. $2'$ 1/4,y,0
4. $2$ x,0,0
5. $1$ (0,0,0)
6. $a$ (1/2,0,0) x,y,0
7. $a$ (1/2,0,0) x,0,z
8. $m'$ 0,y,z
9. $1$ (0,0,0)
10. $a$ (1/2,0,0) x,y,0
11. $m$ x,1/4,z
12. $b'$ (0,1/2,0) 1/4,y,z
13. $1$ (0,0,0)
14. $a$ (1/2,0,0) x,y,0
15. $m$ x,1/4,z
16. $c$ (0,0,1) 0,y,z
17. $1$ (0,0,0)
18. $a$ (1/2,0,0) x,y,0
19. $m$ x,1/4,z
20. $n$ (0,1/2,1) 1/4,y,z

#### For (1/2,1/2,0) + set

1. $t$ (1/2,1/2,1)
2. $2'$ 1/2,0,0
3. $2'$ 0,1/2,0
4. $2$ (1/2,0,0) x,1/4,0
5. $1$ (1/2,1/2,2)
6. $b$ (0,1/2,0) x,y,0
7. $m$ x,1/4,z
8. $b'$ (0,1/2,0) 1/4,y,z
9. $1$ (1/2,1/2,2)
10. $b$ (0,1/2,0) x,y,0
11. $m$ x,1/4,z
12. $c$ (0,0,1) 0,y,z

#### For (0,0,1) + set

1. $t'$ (0,0,1)
2. $2$ (0,0,1) 1/4,0,z
3. $2$ 0,1/2,0
4. $2'$ x,0,1/2
5. $1$ (0,0,1)
6. $a'$ (1/2,0,0) x,y,1/2
7. $n'$ (1/2,0,1) x,0,z
8. $c$ (0,0,1) 0,y,z
9. $1$ (0,0,1)
10. $a'$ (1/2,0,0) x,y,1/2
11. $n'$ (1/2,0,1) x,0,z
12. $m$ (0,0,1)

#### For (1/2,1/2,1) + set

1. $t'$ (1/2,1/2,1)
2. $2$ (0,0,1) 0,1/4,z
3. $2$ (0,1/2,0) 0,y,1/2
4. $2'$ (1/2,0,0) x,1/4,1/2
5. $1$ (1/2,1/2,1)
6. $b'$ (0,1/2,0) x,y,1/2
7. $c'$ (0,0,1) x,1/4,z
8. $n$ (0,1/2,1) 1/4,y,z
9. $1$ (1/2,1/2,1)
10. $b'$ (0,1/2,0) x,y,1/2
11. $c'$ (0,0,1) x,1/4,z
12. $m$ (1/2,1/2,1)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(2) x+1/2, y,z [u,v,w]</td>
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<td>(3) x+1/2, y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 n</td>
<td>m</td>
<td>1/4,0,z [u,v,0]</td>
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<tr>
<td>16 m</td>
<td>m'</td>
<td>1/4,0,z [0,v,0]</td>
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<td>16 l</td>
<td>.2'</td>
<td>3/4,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>16 k</td>
<td>.2</td>
<td>3/4,1,2/1 [u,v,0]</td>
</tr>
<tr>
<td>16 j</td>
<td>.2'</td>
<td>3/4,1,2/0 [u,v,0]</td>
</tr>
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<td>16 i</td>
<td>2'</td>
<td>3/4,1,2/0 [0,v,w]</td>
</tr>
<tr>
<td>16 h</td>
<td>2</td>
<td>3/4,1,2/0 [u,v,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>m'2'</td>
<td>0,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>8 f</td>
<td>.2/m</td>
<td>3/4,1,4/1 [u,v,0]</td>
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<tr>
<td>8 e</td>
<td>.2'/m</td>
<td>3/4,1,4/0 [0,v,0]</td>
</tr>
<tr>
<td>8 d</td>
<td>2'/m'</td>
<td>0,1/2,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 c</td>
<td>2/m'</td>
<td>0,1/2,1/2 [0,v,0]</td>
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<tr>
<td>8 b</td>
<td>2'22'</td>
<td>3/4,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 a</td>
<td>22'2'</td>
<td>3/4,0,0 [u,v,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1'  
\[ a^* = a/2 \quad b^* = b/2 \]
Origin at 0,0,0

Along [1,0,0] p22m2mm  
\[ a^* = -c \quad b^* = b/2 \]
Origin at x,0,0

Along [0,1,0] p2c2mm  
\[ a^* = -a/2 \quad b^* = c \]
Origin at 1/4,y,0
Symmetry Operations

For (0,0,0) + set

(1) \begin{tabular}{c}
1 (1 | 0,0,0) \\
\end{tabular}

(2) \begin{tabular}{c}
2 1/4,0,z (z | 1/2,0,0) \\
\end{tabular}

(3) \begin{tabular}{c}
2' 1/4,y,0 (2z | 1/2,0,0') \\
\end{tabular}

(4) \begin{tabular}{c}
2' x,0,0 (2z | 0,0,0') \\
\end{tabular}

(5) \begin{tabular}{c}
\(\bar{1}\) 0,0,0 \\
(\(\bar{1}\) | 0,0,0) \\
\end{tabular}

(6) \begin{tabular}{c}
a (1/2,0,0) x,y,0 (mz | 1/2,0,0) \\
\end{tabular}

(7) \begin{tabular}{c}
a' (1/2,0,0) x,0,z (mz | 1/2,0,0') \\
\end{tabular}

(8) \begin{tabular}{c}
m' 0,y,z (mz | 0,0,0') \\
\end{tabular}

For (1/2,1/2,0) + set

(1) \begin{tabular}{c}
t (1/2,1/2,0) (1 | 1/2,1/2,0) \\
\end{tabular}

(2) \begin{tabular}{c}
2 0,1/4,z (2z | 1/2,0,0) \\
\end{tabular}

(3) \begin{tabular}{c}
2' (0,1/2,0) 0,y,0 (2z | 0,1/2,0') \\
\end{tabular}

(4) \begin{tabular}{c}
2' (1/2,0,0) x,1/4,0 (2z | 1/2,1/2,0') \\
\end{tabular}

(5) \begin{tabular}{c}
\(\bar{1}\) 1/4,1/4,0 (\(\bar{1}\) | 1/2,1/2,0) \\
\end{tabular}

(6) \begin{tabular}{c}
b (0,1/2,0) x,y,0 (mz | 0,1/2,0) \\
\end{tabular}

(7) \begin{tabular}{c}
m' x,1/4,z (mz | 0,1/2,0) \\
\end{tabular}

(8) \begin{tabular}{c}
b' (0,1/2,0) 1/4,y,z (mz | 1/2,1/2,0) \\
\end{tabular}

For (0,0,1') + set

(1) \begin{tabular}{c}
t' (0,0,1) (1 | 0,0,1') \\
\end{tabular}

(2) \begin{tabular}{c}
2' (0,0,1) 1/4,0,z (2z | 1/2,0,1') \\
\end{tabular}

(3) \begin{tabular}{c}
2 1/4,y,1/2 (2z | 1/2,0,1) \\
\end{tabular}

(4) \begin{tabular}{c}
2 x,0,1/2 (2z | 0,0,1) \\
\end{tabular}

(5) \begin{tabular}{c}
\(\bar{1}\) 0,0,1/2 (\(\bar{1}\) | 0,0,1') \\
\end{tabular}

(6) \begin{tabular}{c}
a' (1/2,0,0) x,y,1/2 (mz | 1/2,0,1) \\
\end{tabular}

(7) \begin{tabular}{c}
n (1/2,0,1) x,0,z (mz | 1/2,0,1) \\
\end{tabular}

(8) \begin{tabular}{c}
c (0,0,1) 0,y,z (mz | 0,0,1) \\
\end{tabular}

For (1/2,1/2,1') + set

(1) \begin{tabular}{c}
t' (1/2,1/2,1) (1 | 1/2,1/2,1') \\
\end{tabular}

(2) \begin{tabular}{c}
2' (0,0,1) 0,1/4,z (2z | 0,1/2,1) \\
\end{tabular}

(3) \begin{tabular}{c}
2 (0,1/2,0) 0,y,1/2 (2y | 0,1/2,1) \\
\end{tabular}

(4) \begin{tabular}{c}
2 (1/2,0,0) x,1/4,1/2 (2x | 1/2,1/2,1) \\
\end{tabular}

(5) \begin{tabular}{c}
\(\bar{1}\) 1/4,1/4,1/2 (\(\bar{1}\) | 1/2,1/2,1') \\
\end{tabular}

(6) \begin{tabular}{c}
b' (0,1/2,0) x,y,1/2 (mz | 0,1/2,1) \\
\end{tabular}

(7) \begin{tabular}{c}
c (0,0,1) x,1/4,z (mz | 0,1/2,1) \\
\end{tabular}

(8) \begin{tabular}{c}
n (0,1/2,1) 1/4,y,z (mz | 1/2,1/2,1) \\
\end{tabular}
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); t(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x + 1/2, y + z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x + 1/2, y, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x, y, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u,v,w]</td>
</tr>
<tr>
<td>16 n .m'</td>
<td>x,1/4,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,1/4,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>0, y, z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,1/4,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,3/4,z [u,v,w]</td>
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<tr>
<td>16 m ..</td>
<td>1/4,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,z [0,0,w]</td>
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<tr>
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<td>1/4,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>16 l ..2</td>
<td>1/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,1/2 [0,0,0]</td>
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<td></td>
<td>1/4,1/2,1/2 [0,0,0]</td>
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<td>1/4,0,1/2 [0,0,0]</td>
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<td>3/4,1/2,1/2 [0,0,0]</td>
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<tr>
<td></td>
<td>1/4,1/2,1/2 [0,0,0]</td>
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<td>16 j .2'</td>
<td>1/4,0,1/2 [0,0,0]</td>
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<td>1/4,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>16 i .2'</td>
<td>1/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,1/2 [0,0,0]</td>
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<td></td>
<td>1/4,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>16 h .2'</td>
<td>1/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,1/2 [0,0,0]</td>
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<td></td>
<td>1/4,1/2,1/2 [0,0,0]</td>
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<tr>
<td>8 g m'm'2</td>
<td>0,1/4,z [0,0,w]</td>
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<td></td>
<td>0,1/4,z [0,0,w]</td>
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<tr>
<td>8 f .2/m'</td>
<td>1/4,1,1/2 [0,0,0]</td>
</tr>
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<td>3/4,1,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 e .2'/m'</td>
<td>1/4,1,1/2 [0,0,0]</td>
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<td>3/4,1,1/2 [0,0,0]</td>
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<tr>
<td>8 d 2/m'..</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
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<tr>
<td>8 c 2'/m'..</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 b 222</td>
<td>1/4,0,1/2 [0,0,0]</td>
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<tr>
<td></td>
<td>3/4,1,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 a 2'2'2</td>
<td>1/4,0,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p2mm1'  
  \[ a^* = a/2 \quad b^* = b/2 \]
- **Along [1,0,0]**: \( p_{2a}2m'm' \)  
  \[ a^* = -c \quad b^* = b/2 \]
- **Along [0,1,0]**: \( p_{2a}2m'm' \)  
  \[ a^* = c \quad b^* = a/2 \]

Origin at 0,0,z  
Origin at x,0,1/2  
Origin at 0,y,1/2
Origin at center (2/m') at 2/m'2'/m2'/a

Asymmetric unit

0 ≤ x ≤ 1/2;

0 ≤ y ≤ 1/4;

0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(5) T
0,0,0

(1|0,0,0)'

(6) a (1/2,0,0) x,y,0

(7) a (1/2,0,0) x,0,z

(8) m' 0,y,z

(1|0,0,0)'

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(1|1/2,1/2,0)'

(5) T
1/4,1/4,0

(1|1/2,1/2,0)'

(2) 2 0,1/4,z

(2|0,1/2,0)

(6) b' (0,1/2,0) x,y,0

(7) m' x,1/4,z

(8) b (0,1/2,0) 1/4, y,z

(2|0,1/2,0)'

(3) 2' (1/2,0,0) 0,y,0

(2|0,1/2,0)'

(4) 2' (1/2,0,0) x,1/4,0

(2|1/2,1/2,0)'

(4) 2 x,0,0

(2|0,0,0)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>o</td>
</tr>
<tr>
<td>8</td>
<td>n</td>
</tr>
<tr>
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<td>j</td>
</tr>
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<td>i</td>
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<td>d</td>
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<td>4</td>
<td>c</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p_{2a}2m'm'</th>
<th>Along [1,0,0] p_{2a}2m'm'</th>
<th>Along [0,1,0] p_{2a}2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a/2</td>
<td>b* = b/2</td>
<td>a* = -a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
C_{pmm'a}  
67.14.590  

Ortorhombic  

mmm1'  
C_{p2'/m2/m'2'}/a  

Origin  at center (2'/m) at 2'/m2/a'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) \(1\)  
\(1\mid 0,0,0\)

(2) \(2\)'  
\(1/4,0,z\)
\((2_x\mid 1/2,0,0)\')

(3) \(2\)  
\(1/4,y,0\)
\((2_y\mid 1/2,0,0)\)

(4) \(2\)'  
\(x,0,0\)
\((2_x\mid 0,0,0)\')

(5) \(\bar{1}\)  
\(0,0,0\)
\((\bar{1}\mid 0,0,0)\')

(6) a (1/2,0,0)  
x,y,0
\((m_z\mid 1/2,0,0)\)

(7) a' (1/2,0,0)  
x,0,z
\((m_y\mid 1/2,0,0)\')

(8) \(m\)  
0,y,z
\((m_x\mid 0,0,0)\)

For (1/2,1/2,0)' + set

(1) \(t\)' (1/2,1/2,0)  
\(1\mid 1/2,1/2,0)\')

(2) \(2\)  
0,1/4,z
\((2_x\mid 0,1/2,0)\)

(3) \(2\)' (0,1/2,0)  
0,y,0
\((2_y\mid 0,1/2,0)\')

(4) \(2\)' (1/2,0,0)  
x,1/4,0
\((2_x\mid 1/2,1/2,0)\)

(5) \(\bar{1}\)  
1/4,1/4,0
\((\bar{1}\mid 1/2,1/2,0)\)

(6) b' (0,1/2,0)  
x,y,0
\((m_z\mid 0,1/2,0)\')

(7) m  
x,1/4,z
\((m_y\mid 0,1/2,0)\)

(8) b' (0,1/2,0)  
1/4,y,z
\((m_x\mid 1/2,1/2,0)\)'
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 o 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 n.m.</td>
<td>x,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>8 m m..</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 l .2'</td>
<td>1/4,0,z [u,v,0]</td>
</tr>
<tr>
<td>8 k .2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 j .2.</td>
<td>1/4,y,0 [0,v,0]</td>
</tr>
<tr>
<td>8 i 2'..</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>8 h 2'..</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>4 g mm2</td>
<td>0,1/4,z [0,0,0]</td>
</tr>
<tr>
<td>4 f .2/m.</td>
<td>1/4,1/4,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 e .2/m.</td>
<td>1/4,1/4,0 [0,v,0]</td>
</tr>
<tr>
<td>4 d 2'm..</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c 2'm..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2'2'</td>
<td>1/4,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 a 2'2'</td>
<td>1/4,0,0 [0,v,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p_{2a}2mm  
  \( a^* = a/2 \quad b^* = b/2 \)  
- Along [1,0,0] p_{2mm}1'  
  \( a^* = b/2 \quad b^* = c \)  
- Origin at 0,0,z  
- Along [0,1,0] p_{2mm}1'  
  \( a^* = c \quad b^* = a/2 \)  
- Origin at x,0,0  
- Origin at 0,y,0
Origin at center (2'/m) at 2'/m2'/a'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For \((0,0,0) +\) set

\[
\begin{align*}
(1) & \quad 1 \\
(1 & |0,0,0) \\
(2) & \quad 2 \quad 1/4, 0, z \\
(2 &_z |1/2, 0, 0) \\
(3) & \quad 2' \quad 1/4, y, 0 \\
(2 &'_z |1/2, 0, 0)' \\
(4) & \quad 2' \quad x, 0, 0 \\
(2 &'_x |0, 0, 0)' \\
(5) & \quad \overline{1} \quad 0, 0, 0 \\
(1 & |0,0,0) \\
(6) & \quad a' \quad (1/2, 0, 0) \quad x, y, 0 \\
(1 & |2, 0, 0)' \\
(7) & \quad a \quad (1/2, 0, 0) \quad x, 0, z \\
(1 & |2, 0, 0)' \\
(8) & \quad m \quad 0, y, z \\
(1 & |2, 0, 0)' \\
\end{align*}
\]

For \((1/2,1/2,0) +\) set

\[
\begin{align*}
(1) & \quad t' \quad (1/2, 1/2, 0) \\
(1 & |1/2, 1/2, 0)' \\
(2) & \quad 2' \quad 0, 1/4, z \\
(2 &_z |0, 1/2, 0)' \\
(3) & \quad 2 \quad (0, 1/2, 0) \quad 0, y, 0 \\
(2 & |0, 1/2, 0) \\
(4) & \quad 2 \quad (1/2, 0, 0) \quad x, 1/4, 0 \\
(2 & |1/2, 1/2, 0) \\
(5) & \quad \overline{1} \quad 1/4, 1/4, 0 \\
(1 & |1/2, 1/2, 0) \\
(6) & \quad b \quad (0, 1/2, 0) \quad x, y, 0 \\
(1 & |2, 0, 0)' \\
(7) & \quad m' \quad x, 1/4, z \\
(1 & |2, 0, 0)' \\
(8) & \quad b' \quad (0, 1/2, 0) \quad 1/4, y, z \\
(1 & |2, 0, 0)' \\
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 o 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>8 n .m'</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>8 m .m..</td>
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<tr>
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<tr>
<td>8 k .2'</td>
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<tr>
<td>8 j .2'</td>
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<tr>
<td>8 i .2'</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>8 h .2'</td>
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<tr>
<td>4 g mm'2</td>
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<tr>
<td>4 f .2'/m'</td>
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<td>4 e .2'/m'</td>
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<tr>
<td>4 d .2'/m'</td>
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<tr>
<td>4 c .2'/m'</td>
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<tr>
<td>4 a .2'2</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2a.2mm

a* = -b/2 b* = a/2
Origin at 0,0,z

Along [1,0,0] p2mm1'

a* = b/2 b* = c
Origin at x,0,0

Along [0,1,0] p2a.2mm

a* = -a/2 b* = c
Origin at 0,y,0
Origin at center (2/m) at 2'/m2/a'a

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $t (0,0,0)$
   1. $1 (0,0,0)$
   2. $2^{'} 1/4,0,z$
      $(2z_{1/2,0,0})$
   3. $2 1/4,y,0$
      $(2y_{1/2,0,0})$
   4. $2^{'} x,0,0$
      $(2x_{0,0,0})$

5. $\bar{1}^{'} 0,0,0$
   $(\bar{1} 0,0,0)_{1/2}$

6. $a (1/2,0,0)_{1/2}$
   $(m_{x} 1/2,0,0)$

7. $a^{'} (1/2,0,0)_{1/2}$
   $(m_{y} 1/2,0,0)$

8. $m_{0,y,z} (m_{z} 0,0,0)$

For $(1/2,1/2,0)$ + set

1. $t^{'} (1/2,1/2,0)_{1/2}$
   1. $t^{'} (1/2,1/2,0)_{1/2}$
   2. $2 0,1/4,z$
      $(2z_{0,1/2,0})$
   3. $2^{'} (0,1/2,0)$
      $(2y_{0,1/2,0})$
   4. $2 (1/2,0,0)_{1/2}$
      $(2x_{1/2,1/2,0})$

5. $\bar{1} 1/4,1/4,0$
   $(\bar{1} 1/2,1/2,0)$

6. $b^{'} (0,1/2,0)_{1/2}$
   $(m_{z} 0,1/2,0)$

7. $m^{'} x,1/4,z$
   $(m_{z} 0,1/2,0)$

8. $b^{'} (0,1/2,0)_{1/2}$
   $(m_{z} 1/2,1/2,0)$

For $(0,0,1)$ + set

1. $t^{'} (0,0,1)_{1/2}$
   1. $t^{'} (0,0,1)_{1/2}$
   2. $2 (0,0,1)_{1/2}$
      $(2z_{1/2,0,1})$
   3. $2^{'} (0,1/2,0)_{1/2}$
      $(2y_{1/2,0,1})$
   4. $2 x,0,1/2$
      $(2x_{0,0,1})$

5. $\bar{1} 0,0,1/2$
   $(\bar{1} 0,0,1)$

6. $a^{'} (1/2,0,0)_{1/2}$
   $(m_{x} 1/2,0,1)$

7. $n (1/2,0,1)_{1/2}$
   $(m_{x} 1/2,0,1)$

8. $c^{'} (0,0,1)_{1/2}$
   $(m_{z} 0,0,1)$

For $(1/2,1/2,1)$ + set

1. $t (1/2,1/2,1)_{1/2}$
   1. $t (1/2,1/2,1)_{1/2}$
   2. $2^{'} (0,0,1)_{1/2}$
      $(2z_{0,1/2,1})$
   3. $2 (0,1/2,0)_{1/2}$
      $(2y_{0,1/2,1})$
   4. $2^{'} (1/2,0,0)_{1/2}$
      $(2x_{1/2,1/2,1})$

5. $\bar{1}^{'} 1/4,1/4,1/2$
   $(\bar{1} 1/2,1/2,1)_{1/2}$

6. $b^{'} (0,1/2,0)_{1/2}$
   $(m_{z} 0,1/2,1)$

7. $c^{'} (0,0,1)_{1/2}$
   $(m_{x} 0,1/2,1)$

8. $n (0,1/2,1)_{1/2}$
   $(m_{z} 1/2,1/2,1)$
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
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<td>(1/2,1/2,0)' +</td>
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<tr>
<td>(0,0,1)'</td>
<td>(1/2,1/2,1) +</td>
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</tbody>
</table>

32 o 1  (1) x,y,z [u,v,w]  (2) x+1/2, y,z [u,v,w]  (3) x+1/2, y,z [u,v,w]  (4) x, y,z [u,v,w]  (5) x, y,z [u,v,w]  (6) x+1/2, y,z [u,v,w]  (7) x+1/2, y,z [u,v,w]  (8) x, y,z [u,v,w]

16 n m..  x,1/4,z [0,v,0]  x,1/4,z [0,v,0]  x,1/4,z [0,v,0]  x,3/4,z [0,v,0]  x,3/4,z [0,v,0]  x,3/4,z [0,v,0]  x,3/4,z [0,v,0]

16 m m..  0,y,z [u,0,0]  0, y+1/2, z [u,0,0]  0, y+1/2, z [u,0,0]  0, y-z [u,0,0]

16 l 2'  1/4,0,z [u,v,0]  3/4,1/2,z [u,v,0]  3/4,1/2,z [u,v,0]  1/4,1/2,z [u,v,0]  1/4,1/2,z [u,v,0]  1/4,1/2,z [u,v,0]  1/4,1/2,z [u,v,0]

16 k 2'  1/4,y,1/4 [u,0,w]  3/4,y+1/2,1/2 [u,0,w]  3/4,y+1/2,1/2 [u,0,w]  1/4,y+1/2,1/2 [u,0,w]  1/4,y+1/2,1/2 [u,0,w]  1/4,y+1/2,1/2 [u,0,w]  1/4,y+1/2,1/2 [u,0,w]

16 j 2'  1/4,y,0 [v,0,0]  3/4,y+1/2,0 [v,0,0]  3/4,y+1/2,0 [v,0,0]  1/4,y+1/2,0 [v,0,0]  1/4,y+1/2,0 [v,0,0]  1/4,y+1/2,0 [v,0,0]  1/4,y+1/2,0 [v,0,0]

16 i 2'  x,0,1/2 [u,0,0]  x,1/2,1/2 [u,0,0]  x,1/2,1/2 [u,0,0]  x,1/2,1/2 [u,0,0]

16 h 2'  x,0,0 [v,w]  x,1/2,0 [v,w]  x,1/2,0 [v,w]  x,1/2,0 [v,w]  x,1/2,0 [v,w]  x,1/2,0 [v,w]  x,1/2,0 [v,w]

8 g mm2  0,1/4,z [0,0,0]  0,3/4,z [0,0,0]  0,3/4,z [0,0,0]

8 f 2'm.  1/4,1/4,1/2 [0,0,0]  3/4,1,4,1/2 [0,0,0]  3/4,1,4,1/2 [0,0,0]

8 e 2'm.  1/4,1/4,0 [0,v,0]  3/4,1,4,0 [0,v,0]  3/4,1,4,0 [0,v,0]

8 d 2'm..  0,0,1/2 [u,0,0]  0,1/2,1/2 [u,0,0]  0,1/2,1/2 [u,0,0]  0,1/2,1/2 [u,0,0]

8 c 2'm..  0,0,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]

8 b 22'2'  1/4,0,1/2 [u,0,0]  3/4,0,1/2 [u,0,0]  3/4,0,1/2 [u,0,0]  3/4,0,1/2 [u,0,0]

8 a 22'2'  1/4,0,0 [v,0,0]  3/4,0,0 [v,0,0]  3/4,0,0 [v,0,0]  3/4,0,0 [v,0,0]

Symmetry of Special Projections

Along [0,0,1]  p2mm1'  Along [1,0,0]  p2mm1'  Along [0,1,0]  p2mm1'

a* = a/2  b* = b/2

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
**CI m'ma'**

**Orthorhombic**

67.17.593

**mmm1'**

C\_1, 2\_m'2/m2'/a'

**Origin**

at center (2'/m') at 2'/m'2'/aa'

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

1. (1) 1
   (1 0,0,0)

2. (2)' 1/4,0,z
   (2\_z 1/2,0,0)'

3. (3) 2' 1/4,y,0
   (2\_y 1/2,0,0)

4. (4) 2' x,0,0
   (2\_x 0,0,0)'

5. (5) 1/2,0,0,0
   (1/2 0,0,0,0)'

6. (6) a'(1/2,0,0) x,y,0
   (m\_z 1/2,0,0)'

7. (7) a(1/2,0,0) x,0,z
   (m\_y 1/2,0,0)'

8. (8) m' 0,y,z
   (m\_x 0,0,0)'

For (1/2,1/2,0)' + set

1. (1) 1/2,1/2,1,0
   (1/2 1/2,1,0,0)'

2. (2) 2 0,1/4,z
   (2\_z 0,1/2,0,0)

3. (3)' 1/2,0,1,0
   (2\_y 1/2,0,1,0)'

4. (4) 1/2,0,0,0
   (2\_x 1/2,1,2,0)'

5. (5) 1/2,1/2,0,0
   (1/2 1/2,0,0,0)'

6. (6) b(0,1/2,0) x,y,0
   (m\_z 0,1/2,0,0)'

7. (7) m' x,1/4,z
   (m\_y 0,1/2,0,0)'

8. (8) b(0,1/2,0) 1/4,y,z
   (m\_z 1/2,1,2,0)'

For (0,0,1)'+ set

1. (1) 0,0,1,0
   (0,0,1,0)'

2. (2) 1/4,0,z
   (1/2 1/2,0,1)

3. (3) 1/4,y,1/2
   (2\_y 1/2,0,1,1)'

4. (4) x,0,1/2
   (2\_x 0,0,1,1)'

5. (5) 0,0,1/2
   (0,0,1/2)'

6. (6) a(1/2,0,0) x,y,1/2
   (m\_z 1/2,0,1)'

7. (7) n'(1/2,0,1) x,0,z
   (m\_y 1/2,0,1,1)'

8. (8) c(0,0,1) 0,y,z
   (m\_x 0,0,1,1)'

For (1/2,1/2,1) + set

1. (1) 1/2,1/2,1,0
   (1/2 1/2,1,0,0)'

2. (2) 0,1/4,z
   (2\_z 0,1/2,1)

3. (3) 0,y,1/2
   (2\_y 0,1/2,1,1)'

4. (4) x,1/4,1/2
   (2\_x 1/2,1,2,1)'

5. (5) 1/4,0,1/2
   (1/2 1/2,0,1)'

6. (6) b'(0,1/2,0) x,y,1/2
   (m\_z 0,1/2,1,1)'

7. (7) c(0,0,1) x,1/4,z
   (m\_y 1/2,0,1,2)'

8. (8) n'(0,1/2,1) 1/4,y,z
   (m\_x 1/2,1/2,1)'

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**Generators selected**  (1); t(1,0,0); t(0,1,0); t'(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

**Positions**

<table>
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<tr>
<th>Multiplicity</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>(1/2,1/2,0) +</td>
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<tr>
<td>(0,0,1) ' +</td>
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<tr>
<th>Positions</th>
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<tbody>
<tr>
<td>32 o 1</td>
<td>(1) x,y,z [u,v,w] (2) x+1/2, y,z [u,v,w] (3) x+1/2,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w]</td>
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<td>x,1/4,z [u,v,w] x,1/4,z [u,v,w] x,1/4,z [u,v,w]</td>
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<tr>
<td>16 m .m':</td>
<td>x,1/4,z [u,v,w] x,1/4,z [u,v,w] x,1/4,z [u,v,w]</td>
</tr>
<tr>
<td>16 l .2'</td>
<td>1/4,0,z [u,v,0] 3/4,1,2, z [u,v,0] 3/4,0, z [u,v,0] 1/4,1,2, z [u,v,0]</td>
</tr>
<tr>
<td>16 k .2'</td>
<td>1/4,y,1/4 [u,v,0] 3/4,y+1/2,1,2 [u,v,0] 3/4,y,1/2 [u,v,0] 1/4,y+1/2,1,2 [u,v,0]</td>
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<tr>
<td>16 j .2'</td>
<td>1/4,y,0 [0,v,0] 3/4,y+1/2,0 [0,v,0] 3/4,y,0 [0,v,0] 1/4,y+1/2,0 [0,v,0]</td>
</tr>
<tr>
<td>16 i .2'</td>
<td>x,0,1/2 [u,v,0] x,1/2,1,2 [u,v,0] x,0,1/2 [u,v,0] x,1/2,1,2 [u,v,0]</td>
</tr>
<tr>
<td>16 h .2'</td>
<td>x,0,0 [0,v,0] x,1,2,0 [0,v,0] x,0,0 [0,v,0] x,1,2,0 [0,v,0]</td>
</tr>
<tr>
<td>8 g m' .m'</td>
<td>0,1/4,z [0,0,0] 0,3/4, z [0,0,0]</td>
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<tr>
<td>8 f .2'm':</td>
<td>1/4,1/4,1,2 [u,v,0] 3/4,1/4,1,2 [u,v,0]</td>
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<tr>
<td>8 e .2'm':</td>
<td>1/4,1/4,0 [0,0,0] 3/4,1/4,0 [0,0,0]</td>
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<tr>
<td>8 d .2'm':</td>
<td>0,0,1/2 [0,0,0] 1/2,1,2 [0,0,0]</td>
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<tr>
<td>8 c .2'm':</td>
<td>0,0,0 [0,0,0]</td>
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<tr>
<td>8 b 22'</td>
<td>1/4,0,1,2 [u,v,0] 3/4,0,1,2 [u,v,0]</td>
</tr>
<tr>
<td>8 a 22'</td>
<td>1/4,0,0,0 [0,0,0] 3/4,0,0,0 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2mm1'
  - $a^* = a/2$  $b^* = b/2$
  - Origin at 0,0,z
- Along [1,0,0] p22mm1'
  - $a^* = b/2$  $b^* = c$
  - Origin at x,0,1/2
- Along [0,1,0] p22mm
  - $a^* = c$  $b^* = a/2$
  - Origin at 1/4,y,0

67.17.593 - 2 - 1177
Ccca

Orthorhombic

68.1.594

mmm

C2/c2/c2/a

Origin at 222 at 2/n2/n2 at 0.1/4.1/4 from \( \bar{T} \)

Asymmetric unit

\( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

For \((0,0,0) + \text{set}\)

\begin{align*}
(1) & \bar{T} \quad 0,1/4,1/4 \\
(5) & 1/2,0,0 \quad x,y,1/4 \\
(6) & b \quad (0,1/2,0) \quad x,y,1/4 \\
(9) & c \quad (0,0,1/2) \quad x,1/4,z \\
(10) & n \quad (0,1/2,1/2) \quad 0,y,z
\end{align*}

For \((1/2,1/2,0) + \text{set}\)

\begin{align*}
(1) & t \quad (1/2,1/2,0) \\
(2) & 1/4,1/4,z \\
(6) & a \quad (1/2,0,0) \quad x,y,1/4 \\
(7) & n \quad (1/2,0,1/2) \quad x,0,z \\
(8) & c \quad (0,0,1/2) \quad 1/4,y,z
\end{align*}
Continued

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

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<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
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<tr>
<td>16 i 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y+1/2,z+1/2 [u,v,w] (6) x,y+1/2,z+1/2 [u,v,w] (7) x,y+1/2,z+1/2 [u,v,w] (8) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 h .2</td>
<td>1/4,1/4,z [0,0,w] 3/4,1/4,z [0,0,w] 3/4,1/4,z+1/2 [0,0,w] 1/4,1/4,z+1/2 [0,0,w]</td>
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<tr>
<td>8 e .2</td>
<td>x,0,0 [u,0,0] x+1/2,1/2,0 [u,0,0] x+1/2,1/2,0 [u,0,0] x+1/2,0,1/2 [u,0,0]</td>
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<td>8 d 1/2</td>
<td>0,1/4,1/4 [u,v,w] 1/2,1/4,1/4 [u,v,w] 1/2,1/4,3/4 [u,v,w] 1/2,1/4,3/4 [u,v,w]</td>
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<tr>
<td>8 c 1/2</td>
<td>1/4,0,1/4 [u,v,w] 1/4,0,1/4 [u,v,w] 3/4,0,3/4 [u,v,w] 3/4,1/2,3/4 [u,v,w]</td>
</tr>
<tr>
<td>4 b 222</td>
<td>0,0,1/2 [0,0,0] 0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 a 222</td>
<td>0,0,0 [0,0,0] 0,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_{c2}2mm</th>
<th>Along [1,0,0]</th>
<th>p_{2a2}2m'm'</th>
<th>Along [0,1,0]</th>
<th>p_{2a2}2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a/2 )</td>
<td>( b^* = b/2 )</td>
<td>( a^* = -c/2 )</td>
<td>( b^* = b/2 )</td>
<td>( a^* = c/2 )</td>
<td>( b^* = a/2 )</td>
</tr>
<tr>
<td>Origin at 1/4,1/4,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Ccca1' Orthorhombic
68.2.595

mmm1' C2/c2/c2/a1'

Origin at 2221' at 2/n2/n2' at 0,1/4,1/4 from 1 1'

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2z | 0,0,0)

(3) 2 0,y,0
(2z' | 0,0,0)

(4) 2 x,0,0
(2z | 0,0,0)

(5) 1' 0,1/4,1/4
(1' | 0,1/2,1/2)

(6) b (0,1/2,0) x,y,1/4
(mz | 0,1/2,1/2)

(7) c (0,0,1/2) x,1/4,z
(my | 0,1/2,1/2)

(8) n (0,1/2,1/2) 0,y,z
(mz | 0,1/2,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 | 1/2,1/2,0)

(2) 2 1/4,1/4,z
(2z' | 1/2,1/2,0)

(3) 2 (0,1/2,0) 1/4,y,0
(2z' | 1/2,1/2,0)

(4) 2 (1/2,0,0) x,1/4,0
(2z | 1/2,1/2,0)

(5) 1' 1/4,0,1/4
(1' | 1/2,0,1/2)

(6) a (1/2,0,0) x,y,1/4
(mz' | 1/2,0,1/2)

(7) n (1/2,0,1/2) x,0,z
(my' | 1/2,0,1/2)

(8) c (0,1/2,1/2) 1/4,y,z
(mz' | 1/2,0,1/2)

For (0,0,0)' + set

(1) t' (1/2,1/2,0)
(1 | 1/2,1/2,0)

(2) 2' 0,0,z
(2z' | 0,0,0)

(3) 2' 0,y,0
(2z' | 0,0,0)

(4) 2' x,0,0
(2z' | 0,0,0)

(5) 1' 0,1/4,1/4
(1' | 0,1/2,1/2)

(6) b' (0,1/2,0) x,y,1/4
(mz' | 0,1/2,1/2)

(7) c' (0,0,1/2) x,1/4,z
(my' | 0,1/2,1/2)

(8) n' (0,1/2,1/2) 0,y,z
(mz' | 0,1/2,1/2)

For (1/2,1/2,0)' + set

(1) t' (1/2,1/2,0)
(1 | 1/2,1/2,0)

(2) 2' 1/4,1/4,z
(2z' | 1/2,1/2,0)

(3) 2' (0,1/2,0) 1/4,y,0
(2z | 1/2,1/2,0)'

(4) 2' (1/2,0,0) x,1/4,0
(2z | 1/2,1/2,0)'

(5) 1' 1/4,0,1/4
(1' | 1/2,0,1/2)

(6) a' (1/2,0,0) x,y,1/4
(mz | 1/2,0,1/2)

(7) n' (1/2,0,1/2) x,0,z
(my | 1/2,0,1/2)

(8) c' (0,0,1/2) 1/4,y,z
(mz | 1/2,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>(0,0,0)' +</td>
<td>(1/2,1/2,0)' +</td>
</tr>
</tbody>
</table>

16 i 11' (1) x,y,z [0,0,0] (2) \(\bar{x},\bar{y},z\) [0,0,0] (3) \(x,\bar{y},z\) [0,0,0] (4) x,y,z [0,0,0] (5) \(\bar{x},\bar{y}+1/2,\bar{z}+1/2\) [0,0,0] (6) x,y+1/2,\(\bar{z}+1/2\) [0,0,0] (7) x,y+1/2,\(z+1/2\) [0,0,0] (8) \(\bar{x},y+1/2,\bar{z}+1/2\) [0,0,0]

8 h ..21' 1/4,1/4,z [0,0,0] 3/4,1/4,\(\bar{z}\) [0,0,0] 3/4,1/4,\(\bar{z}+1/2\) [0,0,0] 1/4,1/4,\(\bar{z}+1/2\) [0,0,0]

8 g ..21' 0,0,z [0,0,0] 0,0,\(\bar{z}\) [0,0,0] 0,1/2,\(\bar{z}+1/2\) [0,0,0] 0,1/2,\(z+1/2\) [0,0,0]

8 f .2.1' 0,y,0 [0,0,0] 1/2,\(\bar{y}+1/2\),0 [0,0,0] 0,\(\bar{y}+1/2,1/2\) [0,0,0] 1/2,\(y+1/2,1/2\) [0,0,0]

8 e 2..1' x,0,0 [0,0,0] \(\bar{x}+1/2,1/2,0\) [0,0,0] \(\bar{x},1/2,1/2\) [0,0,0] x+1/2,0,1/2 [0,0,0]

8 d 1\(\bar{1}\)' 0,1/4,1/4 [0,0,0] 1/2,1/4,1/4 [0,0,0] 0,1/4,3/4 [0,0,0] 1/2,1/4,3/4 [0,0,0]

8 c 1\(\bar{1}\)' 1/4,0,1/4 [0,0,0] 1/4,1/2,1/4 [0,0,0] 3/4,0,3/4 [0,0,0] 3/4,1/2,3/4 [0,0,0]

4 b 2221' 0,0,1/2 [0,0,0] 0,1/2,0 [0,0,0]

4 a 2221' 0,0,0 [0,0,0] 0,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2mm1' Along [1,0,0] p2mm1' Along [0,1,0] p2mm1'

a* = a/2 b* = b/2

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Origin at 22'2' at 2/n'2'/n2' at 0,1/4,1/4 from $\bar{T}$

Asymmetric unit $0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1/2$

Symmetry Operations

For (0,0,0) + set

1. $t (1 | 0,0,0)$
2. $2' 0,0,z (2_z | 0,0,0')$
3. $2' 0,y,0 (2_y | 0,0,0')$
4. $2 x,0,0 (2_x | 0,0,0)$
5. $\bar{T} 0,1/4,1/4 (\bar{T} | 0,1/2,1/2')$
6. $b (0,1/2,0) x,y,1/4 (m_x | 0,1/2,1/2')$
7. $c (0,0,1/2) x,1/4,z (m_y | 0,1/2,1/2')$
8. $n (0,1/2,1/2) 0,y,z (m_z | 0,1/2,1/2')$

For (1/2,1/2,0) + set

1. $t (1/2,1/2,0) (1/2,1/2,0')$
2. $2' 1/4,1/4,z (2_z | 1/2,1/2,0')$
3. $2' (0,1/2,0) 1/4,y,0 (2_y | 1/2,1/2,0')$
4. $2 (1/2,0,0) x,1/4,0 (2_x | 1/2,1/2,0)$
5. $\bar{T} 1/4,0,1/4 (\bar{T} | 1/2,0,1/2')$
6. $a (1/2,0,0) x,y,1/4 (m_z | 1/2,0,1/2)$
7. $n (1/2,0,1/2) x,0,z (m_y | 1/2,0,1/2)$
8. $c' (0,0,1/2) 1/4,y,z (m_z | 1/2,0,1/2')$
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(1/2,1/2,0) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>.2' 1/4,1/4,z [u,v,0]</td>
<td>3/4,1/4,z [u,v,0]</td>
<td>3/4,1/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>.2' 0,0,z [u,v,0]</td>
<td>0,0,z [u,v,0]</td>
<td>0,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 f</td>
<td>.2' 0,y,0 [u,0,w]</td>
<td>1/2,y+1/2,0 [u,0,w]</td>
<td>0,y+1/2,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>2.. x,0,0 [u,0,0]</td>
<td>x+1/2,1/2,0 [u,0,0]</td>
<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 d</td>
<td>1' 0,1/4,1/4 [0,0,0]</td>
<td>1/2,1/4,1/4 [0,0,0]</td>
<td>0,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>8 c</td>
<td>1' 1/4,0,1/4 [0,0,0]</td>
<td>1/4,1/2,1/4 [0,0,0]</td>
<td>3/4,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>22'2' 0,0,1/2 [u,0,0]</td>
<td>0,1/2,0 [u,0,0]</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>22'2' 0,0,0 [u,0,0]</td>
<td>0,1/2,1/2 [u,0,0]</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p22mm  
Along [1,0,0] p222mm  
Along [0,1,0] p2222mm

\begin{align*}
\mathbf{a}^* &= \mathbf{a}/2 & \mathbf{b}^* &= \mathbf{b}/2 & \mathbf{a}^* &= \mathbf{c}/2 & \mathbf{b}^* &= \mathbf{a}/2 \\
\text{Origin at } 0,1/4,z & \quad \text{Origin at } x,0,0 & \quad \text{Origin at } 0,y,1/4
\end{align*}
Origin at 2′2′2 at 2′2′2 at 0,1/4,1/4 from \( \bar{T} \).

Asymmetric unit \( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

**Symmetry Operations**

For \((0,0,0)\) + set

1. \( |\bar{T} \quad 0,1/4,1/4 \)
2. \( |\bar{T} \quad 0,1/2,1/2 \)
3. \( |\bar{T} \quad 1/4,0,1/4 \)
4. \( |\bar{T} \quad 1/2,0,1/2 \)

**Symmetry Operations**

For \((1/2,1/2,0)\) + set

1. \( |\bar{T} \quad 0,1/2,0 \)
2. \( |\bar{T} \quad 1/4,1/4,2 \)
3. \( |\bar{T} \quad 1/2,1/2,0 \)
4. \( |\bar{T} \quad 1/2,0,1/2 \)

**Symmetry Operations**

For \((1/2,1/2,0)\) + set

1. \( |\bar{T} \quad 0,1/2,0 \)
2. \( |\bar{T} \quad 1/4,1/4,2 \)
3. \( |\bar{T} \quad 1/2,1/2,0 \)
4. \( |\bar{T} \quad 1/2,0,1/2 \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>16 i 1</td>
<td>x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y+1/2,z+1/2 [u,v,w] (6) x,y+1/2,z+1/2 [u,v,w] (7) x,y+1/2,z+1/2 [u,v,w] (8) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 h .2</td>
<td>1/4,1/4,z [0,0,w] 3/4,1/4,z [0,0,w] 3/4,1/4,z+1/2 [0,0,w] 1/4,1/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 g .2</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w] 0,1/2,z+1/2 [0,0,w] 0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 f .2'</td>
<td>0,y,0 [u,0,w] 1/2,y+1/2,0 [u,0,w] 0,y+1/2,1/2 [u,0,w] 1/2,y+1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 e 2'..</td>
<td>x,0,0 [v,w] x+1/2,1/2,0 [v,w] x,1/2,1/2 [v,w] x+1/2,0,1/2 [v,w]</td>
</tr>
<tr>
<td>8 d 2'</td>
<td>0,1/4,1/4 [0,0,0] 1/2,1/4,1/4 [0,0,0] 0,1/4,3/4 [0,0,0] 1/2,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>8 c 2'</td>
<td>1/4,0,1/4 [0,0,0] 1/4,1/2,1/4 [0,0,0] 3/4,0,3/4 [0,0,0] 3/4,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2'2'</td>
<td>0,0,1/2 [0,0,w] 0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 a 2'2'</td>
<td>0,0,0 [0,0,w] 0,1/2,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm
  - \( a^* = a/2 \) \( b^* = b/2 \)
- Along [1,0,0] \( p_{2\alpha}2m'm' \)
  - \( a^* = -c/2 \) \( b^* = b/2 \)
- Along [0,1,0] \( p_{2\alpha}2m'm' \)
  - \( a^* = c/2 \) \( b^* = a/2 \)
- Origin at 0,0,z
  - Origin at x,0,1/4
- Origin at 0,1/4,0
### Origin
at $2'2'2'$ at $2'n'2'\!/n'2'\!$ at $0,1/4,1/4$ from $\bar{1}$

### Asymmetric unit
$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

### Symmetry Operations

#### For $(0,0,0)$ + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Matrix</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>$(1</td>
<td>0,0,0)$</td>
</tr>
<tr>
<td>(2) 2</td>
<td>$(2_1</td>
<td>0,0,0)$</td>
</tr>
<tr>
<td>(3) $2'$</td>
<td>$(2'_1</td>
<td>0,0,0)'$</td>
</tr>
<tr>
<td>(4) $2'$</td>
<td>$(2_{1.0,0})$</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td>(5) $\bar{1}$</td>
<td>$(\bar{1}</td>
<td>0,1/4,1/4)$</td>
</tr>
<tr>
<td>(6) $b$</td>
<td>$(0,1/2,0)$</td>
<td>$x,y,1/4$</td>
</tr>
<tr>
<td>(7) $c$</td>
<td>$(0,0,1/2)$</td>
<td>$x,1/4,z$</td>
</tr>
<tr>
<td>(8) $n$</td>
<td>$(0,1/2,1/2)$</td>
<td>$0,y,z$</td>
</tr>
</tbody>
</table>

#### For $(1/2,1/2,0)$ + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Matrix</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $t$</td>
<td>$(1/2,1/2,0)$</td>
<td>$1/4,1/4,z$</td>
</tr>
<tr>
<td>(2) 2</td>
<td>$(2_1</td>
<td>1/2,1/2,0)$</td>
</tr>
<tr>
<td>(3) $2'$</td>
<td>$(2'_1</td>
<td>1/2,1/2,0)'$</td>
</tr>
<tr>
<td>(4) $2'$</td>
<td>$(2_{1.0,0})$</td>
<td>$1/2,0,0$</td>
</tr>
<tr>
<td>(5) $\bar{1}$</td>
<td>$(\bar{1}</td>
<td>1/4,0,1/4)$</td>
</tr>
<tr>
<td>(6) $a$</td>
<td>$(1/2,0,0)$</td>
<td>$x,y,1/4$</td>
</tr>
<tr>
<td>(7) $n'$</td>
<td>$(1/2,0,1/2)$</td>
<td>$x,0,z$</td>
</tr>
<tr>
<td>(8) $c'$</td>
<td>$(0,0,1/2)$</td>
<td>$1/4,0,1/2$</td>
</tr>
</tbody>
</table>

---

**68.5.598 - 1 - 1186**
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>(0,0,0)</td>
<td>(1/2,0,0)</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(1) x+1/2,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(3) x,y,z [u,v,w]</td>
<td>(3) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(5) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(6) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(6) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(8) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(8) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p\text{_}2\text{_}2mm</td>
</tr>
<tr>
<td>a^* = a/2</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>b^* = b/2</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2\text{_}m'</td>
</tr>
<tr>
<td>a^* = -c/2</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>b^* = b/2</td>
<td></td>
</tr>
<tr>
<td>Along [0,1,0]</td>
<td>p2\text{_}m'</td>
</tr>
<tr>
<td>a^* = c/2</td>
<td>Origin at 0,y,0</td>
</tr>
<tr>
<td>b^* = a/2</td>
<td></td>
</tr>
</tbody>
</table>
Origin at 22'2' at 2/n2'/n'2' at 0,1/4,1/4 from \( \bar{1} \)

Asymmetric unit \( 0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \)

Symmetry Operations

For \((0,0,0) + \) set

1. \( \bar{1} \)
   \( (1|0,0,0) \)
2. \( 2' \)
   \( 0,0,z \)
   \( (2_z|0,0,0) \)
3. \( 2' \)
   \( 0,y,0 \)
   \( (2_y|0,0,0) \)
4. \( 2 \)
   \( x,0,0 \)
   \( (2_x|0,0,0) \)
5. \( \bar{1} \)
   \( 0,1/4,1/4 \)
   \( (1|0,1/2,1/2) \)
6. \( b \)
   \( (0,1/2,0) \)
   \( x,y,1/4 \)
   \( (m_z|0,1/2,1/2)' \)
7. \( c \)
   \( (0,0,1/2) \)
   \( x,1/4,z \)
   \( (m_y|0,1/2,1/2)' \)
8. \( n \)
   \( (0,1/2,1/2) \)
   \( 0,y,z \)
   \( (m_x|0,1/2,1/2) \)

For \((1/2,1/2,0) + \) set

1. \( t \)
   \( (1/2,1/2,0) \)
2. \( 2' \)
   \( 1/4,1/4,z \)
   \( (2_z|1/2,1/2,0) \)
3. \( 2' \)
   \( (0,1/2,0) \)
   \( 1/4,y,0 \)
   \( (2_y|1/2,1/2,0) \)
4. \( 2 \)
   \( (1/2,0,0) \)
   \( x,1/4,0 \)
   \( (2_x|1/2,1/2,0) \)
5. \( \bar{1} \)
   \( 1/4,0,1/4 \)
   \( (1|1/2,0,1/2) \)
6. \( a' \)
   \( (1/2,0,0) \)
   \( x,y,1/4 \)
   \( (m_z|1/2,0,1/2)' \)
7. \( n' \)
   \( (1/2,0,1/2) \)
   \( x,0,z \)
   \( (m_y|1/2,0,1/2)' \)
8. \( c \)
   \( (0,0,1/2) \)
   \( 1/4,y,z \)
   \( (m_x|1/2,0,1/2) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>16 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
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<td>(5) x,y+1/2,z+1/2 [u,v,w]</td>
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<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
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<td>(8) x,y+1/2,z+1/2 [u,v,w]</td>
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</table>

8 h ..2' 1/4,1/4,z [u,v,0] 3/4,1/4,z [u,v,0] 3/4,1/4,z+1/2 [u,v,0] 1/4,1/4,z+1/2 [u,v,0]
8 g ..2' 0,0,z [u,v,0] 0,0,z [u,v,0] 0,1/2,z+1/2 [u,v,0] 0,1/2,z+1/2 [u,v,0]
8 f ..2' 0,y,0 [u,0,w] 1/2,y+1/2,0 [u,0,w] 0,y+1/2,1/2 [u,0,w] 1/2,y,1/2 [u,0,w]
8 e .. 0,0,0 [u,0,0] x+1/2,1/2,0 [u,0,0] x+1/2,1/2,0 [u,0,0] x+1/2,0,1/2 [u,0,0]
8 d .. 0,1/4,1/4 [u,v,w] 1/2,1/4,1/4 [u,v,w] 0,1/4,3/4 [u,v,w] 1/2,1/4,3/4 [u,v,w]
8 c .. 1/4,0,1/4 [u,v,w] 1/4,1/2,1/4 [u,v,w] 1/4,0,3/4 [u,v,w] 3/4,1/2,3/4 [u,v,w]
4 b 22'2' 0,0,1/2 [u,0,0] 0,1/2,0 [u,0,0]
4 a 22'2' 0,0,0 [u,0,0] 0,1/2,1/2 [u,0,0]

Symmetry of Special Projections

Along [0,0,1] p2'mm'  Along [1,0,0] p_2m2mm  Along [0,1,0] p2'mm'
a* = a/2  b* = b/2  a* = -c/2  b* = b/2  a* = -a/2  b* = c/2
Origin at 1/4,1/4,z  Origin at x,0,0  Origin at 0,y,0
Origin at 222 at 2/n'2/n'2 at 0,1/4,1/4 from \( \bar{1} \)

Asymmetric unit \( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \quad (1 | 0,0,0) \\
(2) & \quad 2 \quad 0,0,z \quad (2_z | 0,0,0) \\
(3) & \quad 2 \quad y,0 \quad (2_y | 0,0,0) \\
(4) & \quad 2 \quad x,0,0 \quad (2_x | 0,0,0) \\
(5) & \quad \bar{1} \quad 0,1/4,1/4 \quad (\bar{1} | 0,1/2,1/2)' \\
(6) & \quad b \quad (0,1/2,0) \quad x,y,1/4 \quad (m_y | 0,1/2,1/2)' \\
(7) & \quad c \quad (0,0,1/2) \quad x,1/4,z \quad (m_y | 0,1/2,1/2)' \\
(8) & \quad n \quad (0,1/2,1/2) \quad 0,y,z \quad (m_y | 0,1/2,1/2)'
\end{align*}
\]

For \((1/2,1/2,0) + \) set

\[
\begin{align*}
(1) & \quad t \quad (1/2,1/2,2,0) \quad (1 | 1/2,1/2,2,0) \\
(2) & \quad 2 \quad 1/4,1/4,z \quad (2_z | 1/2,1/2,2,0) \\
(3) & \quad 2 \quad (0,1/2,0) \quad 1/4,y,0 \quad (2_y | 1/2,1/2,2,0) \\
(4) & \quad 2 \quad (1/2,0,0) \quad x,1/4,0 \quad (2_x | 1/2,1/2,2,0) \\
(5) & \quad \bar{1} \quad 1/4,0,1/4 \quad (\bar{1} | 1/2,0,1/2)' \\
(6) & \quad a' \quad (1/2,0,0) \quad x,y,1/4 \quad (m_y | 1/2,0,1/2)' \\
(7) & \quad n' \quad (1/2,0,1/2) \quad x,0,z \quad (m_y | 1/2,0,1/2)' \\
(8) & \quad c' \quad (0,0,1/2) \quad 1/4,y,z \quad (m_y | 1/2,0,1/2)'
\end{align*}
\]
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5).

**Positions**

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</tr>
<tr>
<td>8 h .2</td>
<td>1/4,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>8 g .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 f .2</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>8 e .2</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>8 d .1</td>
<td>0,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>8 c .1</td>
<td>1/4,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b 222</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 222</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2m'1m'</th>
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</thead>
<tbody>
<tr>
<td>a* = a/2</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
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<table>
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<tr>
<th>Along [1,0,0]</th>
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<td>a* = b/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
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<table>
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<tr>
<th>Along [0,1,0]</th>
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<tbody>
<tr>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>
Origin at 222 at 2/n2/n2 at 0,1/4,1/4 from \( \overline{1} \)

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For \((0,0,0) + \) set

1. \( \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & z \end{pmatrix} \)
2. \( \begin{pmatrix} 2 & 0 & 0 \\ z & 0 & 0 \end{pmatrix} \)
3. \( \begin{pmatrix} 2 & 0 & y \\ 0 & 0 & 0 \end{pmatrix} \)
4. \( \begin{pmatrix} 2 & x & 0 \\ 0 & 0 & 0 \end{pmatrix} \)
5. \( \begin{pmatrix} \overline{1} & 0 & 1/4, 1/4 \\ 0 & 1/2, 1/2 \end{pmatrix} \)
6. \( \begin{pmatrix} b & (0,1/2,0) \\ 0,1/2,1/2 \end{pmatrix} \)
7. \( \begin{pmatrix} c & (0,0,1/2) \\ 0,1/2,1/2 \end{pmatrix} \)
8. \( \begin{pmatrix} n & (0,1/2,1/2) \\ 0,1/2,1/2 \end{pmatrix} \)

For \((1/2,1/2,0) + \) set

1. \( \begin{pmatrix} t' & (1/2,1/2,0) \\ 1/2,1/2,0 \end{pmatrix} \)
2. \( \begin{pmatrix} 2' & 1/4,1/4,z \\ z & 1/2,1/2,0 \end{pmatrix} \)
3. \( \begin{pmatrix} 2' & (0,1/2,0) \\ z & 1/2,1/2,0 \end{pmatrix} \)
4. \( \begin{pmatrix} 2' & (1/2,0,0) \\ 1/2,1/2,0 \end{pmatrix} \)
5. \( \begin{pmatrix} \overline{1}' & 1/4,0,1/4 \\ 1/2,0,1/2 \end{pmatrix} \)
6. \( \begin{pmatrix} a' & (1/2,0,0) \\ z & 1/2,0,1/2 \end{pmatrix} \)
7. \( \begin{pmatrix} n' & (1/2,0,1/2) \\ 0,0 \end{pmatrix} \)
8. \( \begin{pmatrix} c' & (0,0,1/2) \\ 1/2,0,1/2 \end{pmatrix} \)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

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<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 h ..2'</td>
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</tr>
<tr>
<td>8 d ⊤</td>
<td>0,1/4,1/4 [u,v,w]</td>
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<td>1/4,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b 222</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 222</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a}2m'm'  
\(a^* = -b/2\)  \(b^* = a/2\)
Origin at 0,0,z

Along [1,0,0] p_{2a}2m'm'
\(a^* = b/2\)  \(b^* = c/2\)
Origin at 0,0,0

Along [0,1,0] p2mm
\(a^* = c/2\)  \(b^* = a/2\)
Origin at 0, y, 0
Origin at 22'2' at 2/n2'/n'2' at 0,1/4,1/4 from \( \bar{1} \).

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For \( (0,0,0) \) + set

1. \( 1 \)
   
   \[ (1 \mid 0,0,0) \]

2. \( 2' \quad 0,0,z \)
   
   \[ (2_z \mid 0,0,0)' \]

3. \( 2' \quad 0,y,0 \)
   
   \[ (2 \mid 0,0,0)' \]

4. \( 2 \quad x,0,0 \)
   
   \[ (2_x \mid 0,0,0) \]

5. \( \bar{1} \quad 0,1/4,1/4 \)
   
   \[ (1 \mid 0,1/2,1/2)' \]

6. \( b \quad (0,1/2,0) \)
   
   \[ x,y,1/4 \]

   \[ (m_z \mid 0,1/2,1/2) \]

7. \( c \quad (0,0,1/2) \)
   
   \[ x,1/4,z \]

   \[ (m_y \mid 0,1/2,1/2) \]

8. \( n \quad (0,1/2,1/2) \)
   
   \[ 0,y,z \]

   \[ (m_x \mid 0,1/2,1/2)' \]

For \( (1/2,1/2,0)' \) + set

1. \( t' \quad (1/2,1/2,0) \)
   
   \[ (1/2 \mid 1/2,1/2,0)' \]

2. \( 2 \quad 1/4,1/4,z \)
   
   \[ (2_z \mid 1/2,1/2,0) \]

3. \( 2 \quad (0,1/2,0) \)
   
   \[ 1/4,y,0 \]

   \[ (2_y \mid 1/2,1/2,0) \]

4. \( 2' \quad (1/2,0,0) \)
   
   \[ x,1/4,0 \]

   \[ (2_z \mid 1/2,1/2,0)' \]

5. \( \bar{1} \quad 1/4,0,1/4 \)
   
   \[ (1/2 \mid 1/2,0,1/2)' \]

6. \( a' \quad (1/2,0,0) \)
   
   \[ x,y,1/4 \]

   \[ (m_z \mid 1/2,0,1/2)' \]

7. \( n' \quad (1/2,0,1/2) \)
   
   \[ x,0,z \]

   \[ (m_y \mid 1/2,0,1/2)' \]

8. \( c \quad (0,0,1/2) \)
   
   \[ 1/4,y,z \]

   \[ (m_x \mid 1/2,0,1/2) \]

\[ 68.9.602 - 1 - 1194 \]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>Multiplicity</td>
<td>Coordinates</td>
</tr>
<tr>
<td>Wyckoff letter</td>
<td>Site Symmetry</td>
</tr>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,0)' +</td>
</tr>
<tr>
<td>16 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
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| Symmetry of Special Projections |
|---|---|---|
| Along [0,0,1] | p_{2a}.2mm | Along [1,0,0] | p_{a}.2mm | Along [0,1,0] | p_{c}.2mm |
| a^* = -b/2, b^* = a/2 | a^* = b/2, b^* = c/2 | a^* = c/2, b^* = a/2 |
| Origin at 0,1/4,z | Origin at x,0,0 | Origin at 0,y,1/4 |
Origin at 2'2'2 at 2'/n2'/n'2 at 0,1/4,1/4 from T

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) T (0,0,0) (1) 1
(2) 2 0,0,z (2) 2' 0,0,0
(3) 2' 0,y,0 (3) 2' x,0,0
(4) 2' x,0,0
(5) b (0,1/2,0) (5) 1/4,0,1/4
(6) c (0,0,1/2) (6) b (0,1/2,1/2)
(7) n (0,1/2,1/2) (7) c (0,0,1/2)
(8) n' (0,1/2,1/2) (8) n (0,1/2,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (1) T (1/2,1/2,0)
(2) 2' 1/4,1/4,z (2) 1/2,1/2,0
(3) 2 (0,1/2,0) (3) 2 (0,1/2,0)
(4) 2 (0,1/2,0) (4) 2' 1/4,1/4,0
(5) T 1/4,0,1/4 (5) T 1/2,0,1/2
(6) a (1/2,0,0) (6) a (1/2,0,0)
(7) n' (1/2,0,1/2) (7) n' (1/2,0,1/2)
(8) c' (0,0,1/2) (8) c' (0,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

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<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>16 i 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 h .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 g .2</td>
<td>0,0,z [0,0,w]</td>
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<tr>
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<td>0,0,z [0,0,w]</td>
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<tr>
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<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
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<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 f .2'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y+1/2,0 [u,0,w]</td>
</tr>
<tr>
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<tr>
<td></td>
<td>1/2,y+1/2,0 [u,0,w]</td>
</tr>
<tr>
<td>8 e .2'</td>
<td>x,0,0 [v,w]</td>
</tr>
<tr>
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<td>x+1/2,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td>8 d .1'</td>
<td>0,1/4,1/4 [v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/4,1/4 [v,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/4,3/4 [v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/4,3/4 [v,w]</td>
</tr>
<tr>
<td>8 c .1'</td>
<td>1/4,0,1/4 [v,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,1/2,1/4 [v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,0,3/4 [v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/2,3/4 [v,w]</td>
</tr>
<tr>
<td>4 b 2'2'</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 a 2'2'</td>
<td>0,0,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
</tr>
<tr>
<td>a* = a/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
</tr>
<tr>
<td>a* = b/2</td>
</tr>
<tr>
<td>Origin at x,0,1/4</td>
</tr>
<tr>
<td>Along [0,1,0]</td>
</tr>
<tr>
<td>a* = c/2</td>
</tr>
<tr>
<td>Origin at 1/4,y,1/4</td>
</tr>
</tbody>
</table>
Origin at 22'2' at 2/n2'/n2' at 0,1/4,1/4 from \( \overline{1} \)

Asymmetric unit \( 0 \leq x \leq 1/4; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/2 \)

Symmetry Operations

For \((0,0,0)\) + set

1. \( 1 \)
   \( (1 | 0,0,0) \)

2. \( 2' \ 0,0,z \)
   \( (2_z | 0,0,0)' \)

3. \( 2' \ y,0,0 \)
   \( (2_y | 0,0,0)' \)

4. \( 2 \ x,0,0 \)
   \( (2_x | 0,0,0) \)

5. \( \overline{1} \ 0,1/4,1/4 \)
   \( (\overline{1} | 0,1/2,1/2) \)

6. \( b \ (0,1/2,0) \ x,y,1/4 \)
   \( (m_z | 0,1/2,1/2)' \)

7. \( c \ (0,0,1/2) \ x,1/4,z \)
   \( (m_y | 0,1/2,1/2)' \)

8. \( n \ (0,1/2,1/2) \ 0,y,z \)
   \( (m_y | 0,1/2,1/2) \)

For \((1/2,1/2,0)\) + set

1. \( t' \ (1/2,1/2,0) \)
   \( (1 | 1/2,1/2,0)' \)

2. \( 2 \ 1/4,1/4,z \)
   \( (2_z | 1/2,1/2,0) \)

3. \( 2 \ (0,1/2,0) \ 1/4,y,0 \)
   \( (2_y | 1/2,1/2,0) \)

4. \( 2' \ (1/2,0,0) \ x,1/4,0 \)
   \( (2_x | 1/2,1/2,0)' \)

5. \( \overline{1} \ 1/4,0,1/4 \)
   \( (\overline{1} | 1/2,0,1/2)' \)

6. \( a \ (1/2,0,0) \ x,y,1/4 \)
   \( (m_z | 1/2,0,1/2) \)

7. \( n \ (1/2,0,1/2) \ x,0,z \)
   \( (m_y | 1/2,0,1/2) \)

8. \( c' \ (0,0,1/2) \ 1/4,y,z \)
   \( (m_y | 1/2,0,1/2)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,0); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 i</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0) +</td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(2) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(3) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(4) x,y,z</td>
<td>[u,v,w]</td>
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<tr>
<td>(5) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(6) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(7) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(8) x,y,z</td>
<td>[u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{2a} \cdot 2mm \)  \( a^* = a/2 \)  \( b^* = b/2 \)  \( c^* = c/2 \)
Origin at 1/4,1/4,z

Along [1,0,0] \( p_{cc} \cdot 2mm \)  \( a^* = b/2 \)  \( b^* = c/2 \)  \( a^* = a/2 \)  \( b^* = c/2 \)
Origin at x,0,0

Along [0,1,0] \( p_{2a} \cdot 2m'm' \)  \( a^* = a/2 \)  \( b^* = c/2 \)  \( a^* = a/2 \)  \( b^* = c/2 \)
Origin at 0,y,1/4
Orthorhombic

Asymmetric unit

\[0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \((1 | 0,0,0)\)
2. \((2 | 0,0,z) 0,0,0\)
3. \((3 | 2 \cdot 0,y,0) 2,0,0\)
4. \((4 | 2 \cdot x,0,0) 2,0,0\)
5. \((5 | 1,0,0,0)\)
6. \((6 | m \cdot x,y,0) m,0,0\)
7. \((7 | m \cdot x,0,z) m,0,0\)
8. \((8 | m \cdot 0,y,z) m,0,0\)

For \((0,1/2,1/2) + \text{set}\)

1. \((1 | 1/2,0,1/2)\)
2. \((2 | 2 \cdot 0,0,1/2) 0,0,1/2\)
3. \((3 | 2 \cdot 0,1/2,0) 0,1/2,0\)
4. \((4 | 2 \cdot x,1/4,1/4) 2,x,1/4,1/4\)
5. \((5 | 0,1/4,1/4)\)
6. \((6 | b \cdot 0,1/2,0) 0,1/2,1/2\)
7. \((7 | c \cdot 0,0,1/2) 0,1/2,1/2\)
8. \((8 | n \cdot 0,1/2,1/2) 0,1/2,1/2\)

For \((1/2,0,1/2) + \text{set}\)

1. \((1 | 1/2,0,1/2)\)
2. \((2 | 2 \cdot 0,0,1/2) 1/2,0,1/2\)
3. \((3 | 2 \cdot 1/4,0,1/4) 1/2,0,1/2\)
4. \((4 | 2 \cdot 1/2,0,0) 1/2,0,1/2\)
5. \((5 | 1/2,0,1/2)\)
6. \((6 | a \cdot 1/2,0,0) 1/2,0,1/2\)
7. \((7 | n \cdot 1/2,0,1/2) 1/2,0,1/2\)
8. \((8 | c \cdot 0,1/2,1/2) 1/2,0,1/2\)

For \((1/2,1/2,0) + \text{set}\)

1. \((1 | 1/2,1/2,0)\)
2. \((2 | 2 \cdot 1/4,1/4,0) 1/2,1/2,0\)
3. \((3 | 2 \cdot 0,1/2,0) 1/2,1/2,0\)
4. \((4 | 2 \cdot 1/2,0,0) 1/2,1/2,0\)
5. \((5 | 1/2,1/2,0)\)
6. \((6 | n \cdot 1/2,1/2,0) 1/2,1/2,0\)
7. \((7 | a \cdot 1/2,0,0) 1/2,1/2,0\)
8. \((8 | b \cdot 0,1/2,0) 1/2,1/2,0\)
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5). \)

Positions

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
</tr>
<tr>
<td>32 p 1 (1) ( x,y,z [u,v,w] )</td>
<td>(2) ( \bar{x},y,z [\bar{u},v,\bar{w}] )</td>
</tr>
<tr>
<td>16 o ..m</td>
<td>( x,y,0 [0,0,w] )</td>
</tr>
<tr>
<td>16 n ..m</td>
<td>( x,0,z [0,v,0] )</td>
</tr>
<tr>
<td>16 m ..m</td>
<td>( 0,y,z [u,0,0] )</td>
</tr>
<tr>
<td>16 l ..m</td>
<td>( x,1/4,1/4 [u,0,0] )</td>
</tr>
<tr>
<td>16 k ..m</td>
<td>( 1/4,y,1/4 [0,v,0] )</td>
</tr>
<tr>
<td>16 j ..m</td>
<td>( 1/4,1/4,z [0,0,w] )</td>
</tr>
<tr>
<td>8 i mm2</td>
<td>( 0,0,z [0,0,0] )</td>
</tr>
<tr>
<td>8 h m2m</td>
<td>( 0,y,0 [0,0,0] )</td>
</tr>
<tr>
<td>8 g 2mm</td>
<td>( x,0,0 [0,0,0] )</td>
</tr>
<tr>
<td>8 f 222</td>
<td>( 1/4,1/4,1/4 [0,0,0] )</td>
</tr>
<tr>
<td>8 e ..m</td>
<td>( 1/4,1/4,0 [0,0,w] )</td>
</tr>
<tr>
<td>8 d ..m</td>
<td>( 1/4,0,1/4 [0,v,0] )</td>
</tr>
<tr>
<td>8 c ..m</td>
<td>( 0,1/4,1/4 [u,0,0] )</td>
</tr>
<tr>
<td>4 b mmm</td>
<td>( 0,0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>4 a mmm</td>
<td>( 0,0,0 [0,0,0] )</td>
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</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\] p2mm1' \( a^* = a/2 \) \( b^* = b/2 \) Origin at 0,0,z
Along \([1,0,0]\] p2mm1' \( a^* = b/2 \) \( b^* = c/2 \) Origin at \(x,0,0\)
Along \([0,1,0]\] p2mm1' \( a^* = c/2 \) \( b^* = a/2 \) Origin at 0,\(y,0\)
Fmmm1'  
Orthorhombic  
69.2.606  

Asymmetric unit  
$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
   
   $(1 \mid 0,0,0)$

2. $2$ 0,0,z
   
   $(2_z \mid 0,0,0)$

3. $2$ 0,y,0
   
   $(2_y \mid 0,0,0)$

4. $2$ x,0,0
   
   $(2_x \mid 0,0,0)$

5. $\overline{1}$ 0,0,0
   
   $(\overline{1} \mid 0,0,0)$

6. $m$ x,y,0
   
   $(m_z \mid 0,0,0)$

7. $m$ x,0,z
   
   $(m_y \mid 0,0,0)$

8. $m$ 0,y,z
   
   $(m_x \mid 0,0,0)$

For $(0,1/2,1/2)$ + set

1. $t$ $(0,1/2,1/2)$
   
   $(1 \mid 0,1/2,1/2)$

2. $2$ (0,0,1/2) 0,1/4,z
   
   $(2_z \mid 0,1/2,1/2)$

3. $2$ (0,1/2,0) 0,y,1/4
   
   $(2_y \mid 0,1/2,1/2)$

4. $2$ (1/2,0,0) x,0,1/4
   
   $(2_x \mid 0,1/2,1/2)$

5. $\overline{1}$ 0,1/4,1/4
   
   $(\overline{1} \mid 0,1/2,1/2)$

6. $b$ (0,1/2,0) x,y,1/4
   
   $(m_x \mid 0,1/2,1/2)$

7. $c$ (0,0,1/2) x,1/4,z
   
   $(m_y \mid 0,1/2,1/2)$

8. $n$ (0,1/2,1/2) 0,y,z
   
   $(m_z \mid 0,1/2,1/2)$

For $(1/2,0,1/2)$ + set

1. $t$ $(1/2,0,1/2)$
   
   $(1 \mid 1/2,0,1/2)$

2. $2$ (0,0,1/2) 1/4,0,z
   
   $(2_z \mid 1/2,0,1/2)$

3. $2$ (0,1/2,0) 1/4,y,1/4
   
   $(2_y \mid 1/2,0,1/2)$

4. $2$ (1/2,0,0) x,0,1/4
   
   $(2_x \mid 1/2,0,1/2)$

5. $\overline{1}$ 1/4,0,1/4
   
   $(\overline{1} \mid 1/2,0,1/2)$

6. $a$ (1/2,0,0) x,y,1/4
   
   $(m_x \mid 1/2,0,1/2)$

7. $n$ (1/2,0,1/2) x,0,z
   
   $(m_y \mid 1/2,0,1/2)$

8. $c$ (0,0,1/2) 1/4,y,z
   
   $(m_z \mid 1/2,0,1/2)$

For $(1,2,1,2,0)$ + set

1. $t$ $(1,2,1,2,0)$
   
   $(1 \mid 1/2,1/2,0)$

2. $2$ 1/4,1/4,z
   
   $(2_z \mid 1/2,1/2,0)$

3. $2$ (0,1/2,0) 1/4,y,0
   
   $(2_y \mid 1/2,1/2,0)$

4. $2$ (1/2,0,0) x,1/4,0
   
   $(2_x \mid 1/2,1/2,0)$

5. $\overline{1}$ 1/4,1/4,0
   
   $(\overline{1} \mid 1/2,1/2,0)$

6. $n$ (1,2,1,2,0) x,y,0
   
   $(m_z \mid 1/2,1/2,0)$

7. $a$ (1/2,0,0) x,1/4,z
   
   $(m_y \mid 1/2,1/2,0)$

8. $b$ (0,1/2,0) 1/4,y,z
   
   $(m_z \mid 1/2,1/2,0)$
Continued

For (0,0,0)'+ set

(1) t' (0,0,0)'
   (1) 0,0,0')

(2) 2' 0,0,z
    (2) |0,0,0)'

(3) 2' 0,y,0
    (3) |0,0,0)'

(4) 2' x,0,0
    (4) |0,0,0)'

(5) T' 0,0,0
   (T |0,0,0)'

(6) m' x,y,0
    (6) |0,0,0)'

(7) m' x,0,z
    (7) |0,0,0)'

(8) m' 0,y,z
    (8) |0,0,0)'

For (0,1/2,1/2)'+ set

(1) t' (0,1/2,1/2)
   (1) |0,1/2,1/2)

(2) 2' (0,0,1/2) 0,1/4,z
    (2) |0,1/2,1/2)

(3) 2' (0,1/2,0) y,1/4
    (3) |0,1/2,1/2)

(4) 2' x,1/4,1/4
    (4) |0,1/2,1/2)

(5) T' 0,1/4,1/4
   (T |0,1/2,1/2)

(6) b' (0,1/2,0) x,y,1/4
    (6) |0,1/2,1/2)

(7) c' (0,0,1/2) x,1/4,z
    (7) |0,1/2,1/2)

(8) n' (0,1/2,1/2) 0,y,z
    (8) |0,1/2,1/2)

For (1/2,0,1/2)'+ set

(1) t' (1/2,0,1/2)
   (1) |1/2,0,1/2)

(2) 2' (0,0,1/2) 1/4,0,z
    (2) |1/2,0,1/2)

(3) 2' 1/4,y,1/4
    (3) |1/2,0,1/2)

(4) 2' (1/2,0,0) x,0,1/4
    (4) |1/2,0,1/2)

(5) T' 1/4,0,1/4
   (T |1/2,0,1/2)

(6) a' (1/2,0,0) x,y,1/4
    (6) |1/2,0,1/2)

(7) c' (0,0,1/2) x,1/4,z
    (7) |1/2,0,1/2)

(8) n' (0,1/2,1/2) 0,y,z
    (8) |1/2,0,1/2)

For (1/2,1/2,0)'+ set

(1) t' (1/2,1/2,0)
   (1) |1/2,1/2,0)

(2) 2' 1/4,1/4,z
    (2) |1/2,1/2,0)

(3) 2' (0,1/2,0) 1/4,y,0
    (3) |1/2,1/2,0)

(4) 2' (1/2,0,0) x,1/4,0
    (4) |1/2,1/2,0)

(5) T' 1/4,1/4,0
   (T |1/2,1/2,0)

(6) n' (1/2,1/2,0) x,y,0
    (6) |1/2,1/2,0)

(7) a' (1/2,0,0) x,1/4,z
    (7) |1/2,1/2,0)

(8) b' (0,1/2,0) 1/4,y,z
    (8) |1/2,1/2,0)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5): t'.

Positions

Multiset,
Wyckoff letter,
Site Symmetry.

Multipliciy

Coordinates

(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
(0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)'

32 p 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]
          (5) x,y,z [0,0,0] (6) x,y,z [0,0,0] (7) x,y,z [0,0,0] (8) x,y,z [0,0,0]

16 o _m1' x,y,0 [0,0,0] x,y,0 [0,0,0] x,y,0 [0,0,0] x,y,0 [0,0,0]

16 n _m1' x,0,z [0,0,0] x,0,z [0,0,0] x,0,z [0,0,0] x,0,z [0,0,0]

16 m _m1' 0,y,z [0,0,0] 0,y,z [0,0,0] 0,y,z [0,0,0] 0,y,z [0,0,0]

16 l _1' x,1/4,1/4 [0,0,0] x,1/4,1/4 [0,0,0] x,1/4,1/4 [0,0,0] x,1/4,1/4 [0,0,0]
Continued

<table>
<thead>
<tr>
<th>16 k</th>
<th>.21'</th>
<th>1/4,y,1/4 [0,0,0]</th>
<th>3/4,y,1/4 [0,0,0]</th>
<th>3/4, y,3/4 [0,0,0]</th>
<th>1/4,y,3/4 [0,0,0]</th>
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<tbody>
<tr>
<td>16 j</td>
<td>.21'</td>
<td>1/4,1/4,z [0,0,0]</td>
<td>3/4,1/4,z [0,0,0]</td>
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<td>8 i</td>
<td>mm2 1'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<tr>
<td>8 h</td>
<td>m2 1'</td>
<td>0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
<td>0,y,0 [0,0,0]</td>
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<tr>
<td>8 g</td>
<td>2mm1'</td>
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<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
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<tr>
<td>8 f</td>
<td>2221'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>8 e</td>
<td>..2/m1'</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
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<tr>
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<td>.2/m1'</td>
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<td>3/4,0,1/4 [0,0,0]</td>
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<tr>
<td>8 c</td>
<td>2/m1'</td>
<td>0,1/4,1/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
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<tr>
<td>4 b</td>
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<td>0,0,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>4 a</td>
<td>mmm1'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1'  
Along [1,0,0] p2mm1'  
Along [0,1,0] p2mm1'

\[ a^* = a/2 \quad b^* = b/2 \quad a^* = b/2 \quad b^* = c/2 \quad a^* = c/2 \quad b^* = a/2 \]

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0

69.2.606 - 3 - 1204
**Orthorhombic**

69.3.607

**Symmetry Operations**

**For** $(0,0,0)$ + set

1. $t (0,0,0)$
2. $2' (0,0,0), z$
3. $2' (0,0,0)$
4. $2 (0,0,0)$
5. $m (0,0,0)$
6. $m (0,0,0)$
7. $m' (0,0,0)$
8. $m' (0,0,0)$

**For** $(0,1/2,1/2)$ + set

1. $t (0,1/2,1/2)$
2. $2' (0,1/2,1/2), 0,1/4, z$
3. $2' (0,1/2,1/2), 0,1/4, z$
4. $2 (0,1/2,1/2), 1/4, 0, z$
5. $m (0,1/2,1/2)$
6. $m (0,1/2,1/2)$
7. $m (0,1/2,1/2)$
8. $m (0,1/2,1/2)$

**For** $(1/2,0,1/2)$ + set

1. $t (1/2,0,1/2)$
2. $2' (1/2,0,1/2), 1/4, 0, z$
3. $2' (1/2,0,1/2), 1/4, 0, z$
4. $2 (1/2,0,1/2), 1/4, 0, z$
5. $m (1/2,0,1/2)$
6. $m (1/2,0,1/2)$
7. $m (1/2,0,1/2)$
8. $m (1/2,0,1/2)$

**For** $(1/2,1/2,0)$ + set

1. $t (1/2,1/2,0)$
2. $2' (1/2,1/2,0), 1/4, 0, z$
3. $2' (1/2,1/2,0), 1/4, 0, z$
4. $2 (1/2,1/2,0), 1/4, 0, z$
5. $m (1/2,1/2,0)$
6. $m (1/2,1/2,0)$
7. $m (1/2,1/2,0)$
8. $m (1/2,1/2,0)$

Asymmetric unit: $0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
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<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
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<tr>
<td>32 p 1 (1) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 o .m x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
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<tr>
<td>16 n .m x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
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<tr>
<td>16 m .m' 0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
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<tr>
<td>16 i 2.. x,1/4,1/4 [u,0,0]</td>
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<td>3/4,y,3/4 [u,0,w]</td>
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<tr>
<td>16 j ..2' 1/4,1/4,z [u,v,0]</td>
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<td>0,0,z [0,v,0]</td>
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<tr>
<td>8 h m'2'm 0,y,0 [0,0,w]</td>
<td>0,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 g 2mm x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>8 f 22'2' 1/4,1/4,1/4 [u,0,0]</td>
<td>3/4,3/4,3/4 [u,0,0]</td>
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<tr>
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<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>8 d .2'/m. 1/4,0,1/4 [0,0,0]</td>
<td>3/4,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>8 c 2/m'.. 0,1/4,1/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b m'mm 0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a m'mm 0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm1'  a* = a/2  b* = b/2
- Along [1,0,0] p2mm  a* = b/2  b* = c/2
- Along [0,1,0] p2mm1'  a* = c/2  b* = a/2

Origin at 0,0,z  Origin at x,0,0  Origin at 0,y,0
Orthorhombic

Fm'\text{m}'m' \quad \text{69.4.608} \quad m'm' \quad F2'/m'2'/m'2/m

Origin at center (m'm'm)

Asymmetric unit:

\hspace{1cm} 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2

Symmetry Operations

For (0,0,0) + set:

\begin{align*}
(1) \quad & \text{t} (0,0,0) \\
(2) \quad & 2 (0,0,z) \quad (2z,0,0,0) \\
(3) \quad & 2' (0,y,0) \quad (2z,0,0,0)' \\
(4) \quad & 2' (x,0,0) \quad (2z,0,0,0)'
\end{align*}

For (0,1/2,1/2) + set:

\begin{align*}
(1) \quad & \text{t} (0,1/2,1/2) \\
(2) \quad & 2 (0,0,1/2) \quad 0,1/4,z \\
(3) \quad & 2' (0,1/2,0) \quad 0,y,1/4 \\
(4) \quad & 2' (x,1/4,1/4) \quad (2z,0,1/2,1/2)'
\end{align*}

For (1/2,0,1/2) + set:

\begin{align*}
(1) \quad & \text{t} (1/2,0,1/2) \\
(2) \quad & 2 (0,0,1/2) \quad 1/4,0,z \\
(3) \quad & 2' (1/2,0,0) \quad x,0,1/4 \\
(4) \quad & 2' (1/2,0,0) \quad x,0,1/4
\end{align*}

For (1/2,1/2,0) + set:

\begin{align*}
(1) \quad & \text{t} (1/2,1/2,0) \\
(2) \quad & 2 (0,1/2,0) \quad 1/4,1/4,z \\
(3) \quad & 2' (0,1/2,0) \quad 1/4,y,0 \\
(4) \quad & 2' (1/2,0,0) \quad x,1/4,0
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
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<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
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<td>(0,0,0)</td>
<td>(0,1/2,1/2)</td>
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<td>32 p 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>(5) x,y,z [u,v,w]</td>
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</tr>
<tr>
<td>16 o .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>16 n .m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>16 m .m''</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>16 l .2''</td>
<td>x,1/4,1/4 [0,v,w]</td>
</tr>
<tr>
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<td>1/4,1/4,y [u,0,w]</td>
</tr>
<tr>
<td>16 j .2</td>
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</tr>
<tr>
<td>8 i m'2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 h m'2</td>
<td>0,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 g 2'm'm</td>
<td>x,0,0 [0,0,w]</td>
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<tr>
<td>8 f 2'2'</td>
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<tr>
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<td>0,0,0 [0,0,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'

\[ \mathbf{a}^* = \frac{a}{2} \quad \mathbf{b}^* = \frac{b}{2} \]

Origin at 0,0,z

Along [1,0,0] p2mm'

\[ \mathbf{a}^* = -\frac{c}{2} \quad \mathbf{b}^* = \frac{b}{2} \]

Origin at x,0,0

Along [0,1,0] p2mm'

\[ \mathbf{a}^* = \frac{c}{2} \quad \mathbf{b}^* = \frac{a}{2} \]

Origin at 0,y,0
Origin at center (m'm'm')

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

1. $T (1|0,0,0)$
2. $T (2|0,0,z)$
3. $T (2|0,y,0)$
4. $T (2|x,0,0)$
5. $T (1|0,0,0)'$
6. $T (m'x|0,y,0)$
7. $T (m'x|0,z)$
8. $T (m'0,y,z)$

For (0,1/2,1/2) + set

1. $T (1|0,1/2,1/2)$
2. $T (2|0,0,1/2)$
3. $T (2|0,y,1/4)$
4. $T (2|x,0,0)$
5. $T (1|0,1/2,1/2)'$
6. $T (m'x|0,y,0)$
7. $T (m'x|0,z)$
8. $T (m'0,y,z)$

For (1/2,0,1/2) + set

1. $T (1|1/2,0,1/2)$
2. $T (2|0,1/2,1/2)$
3. $T (2|1/4,y,1/4)$
4. $T (2|x,0,0)$
5. $T (1|1/2,0,1/2)'$
6. $T (m'x|0,y,0)$
7. $T (m'x|0,z)$
8. $T (m'0,y,z)$

For (1,2,0,1/2) + set

1. $T (1|1/2,1/2,0)$
2. $T (2|0,1/2,1/2)$
3. $T (2|1/4,y,1/4)$
4. $T (2|x,0,0)$
5. $T (1|1/2,2,0,1/2)'$
6. $T (m'x|0,y,0)$
7. $T (m'x|0,z)$
8. $T (m'0,y,z)$

For (1/2,1,2,0) + set

1. $T (1|1/2,1/2,0)$
2. $T (2|1/4,y,z)$
3. $T (2|x,0,0)$
4. $T (2|x,1/2,2,0)$
5. $T (1|1/2,1/2,0)'$
6. $T (m'x|0,y,0)$
7. $T (m'x|0,z)$
8. $T (m'0,y,z)$
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

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<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td></td>
</tr>
<tr>
<td>32 p 1 x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>16 o m' x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0]</td>
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</tr>
<tr>
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<tr>
<td>16 m' m' 0,y,z [0,v,w] 0,y,z [0,v,w] 0,y,z [0,v,w]</td>
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<tr>
<td>16 l 2 x,1/4,1/4 [u,0,0] x,3/4,1/4 [u,0,0] x,3/4,3/4 [u,0,0] x,1/4,3/4 [u,0,0]</td>
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</tr>
<tr>
<td>16 j 2 1/4,1/4,z [0,0,w] 3/4,1/4,z [0,0,w] 3/4,3/4,z [0,0,w] 1/4,3/4,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 i m'2 0,0,z [0,0,w] 0,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 h m'2 0,y,0 [0,v,0] 0,y,0 [0,v,0]</td>
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</tr>
<tr>
<td>8 g 2m'1 x,0,0 [u,0,0] x,0,0 [u,0,0]</td>
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<tr>
<td>8 f 222 1/4,1/4,1/4 [0,0,0] 3/4,3/4,3/4 [0,0,0]</td>
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</tr>
<tr>
<td>8 e 2/m' 1/4,1/4,0 [0,0,0] 3/4,1/4,0 [0,0,0]</td>
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</tr>
<tr>
<td>8 d 2/m' 1/4,0,1/4 [0,0,0] 3/4,0,1/4 [0,0,0]</td>
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<tr>
<td>8 c 2/m' 0,1/4,1/4 [0,0,0] 0,3/4,1/4 [0,0,0]</td>
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<tr>
<td>4 b m'm' 0,0,1/2 [0,0,0]</td>
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<tr>
<td>4 a m'm' 0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm' a* = a/2 b* = b/2 Origin at 0,0,z
Along [1,0,0] p2m'm' a* = b/2 b* = c/2 Origin at x,0,0
Along [0,1,0] p2m'm' a* = c/2 b* = a/2 Origin at 0,y,0
**Asymmetric unit**  
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set

1. 1  
   (1) 0,0,0

2. 2  0,0,z  
   (2) z,0,0,0

3. 2  0,y,0  
   (2) 0,0,0

4. 2  x,0,0  
   (2) x,0,0,0

5. 1  0,0,0  
   (5) 0,0,0

6. m  x,y,0  
   (m) x,y,0

7. m  x,0,z  
   (m) x,0,z

8. m  0,y,z  
   (m) 0,y,z

For (0,1/2,1/2) + set

1. t (0,1/2,1/2)  
   (1) 0,1/2,1/2

2. 2  0,0,1/2  
   (2) z,0,1/2,1/2

3. 2  0,1/2,0  
   (2) 0,1/2,1/2

4. 2  x,1/4,1/4  
   (2) x,0,1/2,1/2

5. 1  0,1/4,1/4  
   (5) 0,1/4,1/4

6. m  x,y,1/4  
   (m) x,y,1/4

7. m  x,0,1/4  
   (m) x,0,1/4

8. m  0,y,1/4  
   (m) 0,y,1/4

For (1/2,0,1/2) + set

1. t (1/2,0,1/2)  
   (1) 1/2,0,1/2

2. 2  0,0,1/2  
   (2) z,0,1/2,1/2

3. 2  1/4,0,1/4  
   (2) z,1/2,0,1/2

4. 2  x,0,1/4  
   (2) x,1/2,0,1/2

5. 1  1/4,0,1/4  
   (5) 1/4,0,1/4

6. m  x,y,1/4  
   (m) x,y,1/4

7. m  x,0,1/4  
   (m) x,0,1/4

8. m  0,y,1/4  
   (m) 0,y,1/4

For (1/2,2,0,1/2) + set

1. t (1/2,1,2/0)  
   (1) 1/2,1,2/0

2. 2  1/4,1/4,z  
   (2) z,1/2,1/2,0

3. 2  0,1/2,0  
   (2) 1/2,1/2,0

4. 2  x,1/4,1/4  
   (2) x,1/2,1/2,0

5. t (1/2,1,2/0)  
   (5) 1/2,1,2/0

6. m  x,y,0  
   (m) x,y,0

7. m  x,0,1/4  
   (m) x,0,1/4

8. m  0,y,1/4  
   (m) 0,y,1/4
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
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<tbody>
<tr>
<td>(0,0,0)</td>
<td>(0,1/2,1/2)'</td>
<td>(1/2,0,1/2)'</td>
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<tr>
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<td>(1) x,y,z [u,v,w]</td>
<td>[u,v,w]</td>
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<td>(5) x,y,z</td>
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<td>[0,0,w]</td>
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<td>x,0,z [0,v,0]</td>
<td>[0,v,0]</td>
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<td>0,y,z [u,0,0]</td>
<td>[u,0,0]</td>
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<td>x,1/4,1/4 [0,v,w]</td>
<td>[0,v,w]</td>
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<td>[u,0,w]</td>
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<td>[0,0,0]</td>
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<td>[0,0,w]</td>
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<tr>
<td>4 b mmm</td>
<td>0,0,1/2 [0,0,0]</td>
<td>[0,0,0]</td>
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<tr>
<td>4 a mmm</td>
<td>0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p2mm1' Along [1,0,0] p2mm1' Along [0,1,0] p2mm1'

\[ a^* = a/2 \quad b^* = b/2 \quad a^* = b/2 \quad b^* = c/2 \]

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0

69.6.610 - 2 - 1212
Asymmetric unit: $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
2. $2' \quad 0,0,z$
3. $2' \quad 0,y,0$
4. $2 \quad x,0,0$
5. $1 \quad 0,0,0$
6. $m \quad x,y,0$
7. $m \quad x,0,z$
8. $m' \quad 0,y,z$

For $(0,1/2,1/2)' + set$

1. $t' \quad (0,1/2,1/2)$
2. $2' \quad 0,0,1/2, 1/4,z$
3. $2 \quad (0,1/2,0) \quad 0,y,1/4$
4. $2' \quad x,1/4,1/4$
5. $1 \quad (0,1/2,1/2)'$
6. $b' \quad (0,1/2,0) \quad x,y,1/4$
7. $c' \quad (0,0,1/2) \quad x,1/4,z$
8. $n \quad (0,1/2,1/2) \quad 0,y,z$

For $(1/2,0,1/2) + set$

1. $t' \quad (1/2,0,1/2)$
2. $2 \quad (0,0,1/2) \quad 1/4,0,z$
3. $2 \quad 1/4,y,1/4$
4. $2' \quad (1/2,0,0) \quad x,0,1/4$
5. $1 \quad (1/2,0,1/2)'$
6. $a' \quad (1/2,0,0) \quad x,y,1/4$
7. $n' \quad (1/2,0,1/2) \quad x,0,z$
8. $c \quad (0,0,1/2) \quad 1/4,y,z$

For $(1/2,1/2,0) + set$

1. $t \quad (1/2,1,2,0)$
2. $2' \quad 1/4,1/4,z$
3. $2' \quad (0,1/2,0) \quad 1/4,y,0$
4. $2 \quad (1/2,1/2,0)$
5. $1 \quad (1/2,1,2,0)'
6. $n \quad (1/2,1,2,0) \quad x,y,0$
7. $a \quad (1/2,2,0) \quad x,1/4,z$
8. $b' \quad (0,1/2,0) \quad 1/4,y,z$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>32 p 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,1/2,1/2)' + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td>(0,0,0) + (0,1/2,1/2)' + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>16 o .m</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>16 n .m.</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>16 m m'..</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>16 l 2'..</td>
<td>x,1/4,1/4 [0,v,w]</td>
<td>x,3/4,1/4 [0,v,w]</td>
<td>x,1/4,1/4 [0,v,w]</td>
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<tr>
<td>16 k .2.</td>
<td>1/4,y,1/4 [0,v,0]</td>
<td>3/4,y,3/4 [0,v,0]</td>
<td>1/4,y,3/4 [0,v,0]</td>
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<tr>
<td>16 j .2'</td>
<td>1/4,1/4,z [u,v,0]</td>
<td>3/4,3/4,z [u,v,0]</td>
<td>1/4,3/4,z [u,v,0]</td>
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<tr>
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<td>0,0,z [0,v,0]</td>
<td>0,0,z [0,v,0]</td>
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<tr>
<td>8 h m'2'm</td>
<td>0,y,0 [0,0,w]</td>
<td>0,y,0 [0,0,w]</td>
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<tr>
<td>8 g 2mm</td>
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<tr>
<td>8 e .2' m</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
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<tr>
<td>8 d .2/m.</td>
<td>1/4,0,1/4 [0,v,0]</td>
<td>3/4,0,1/4 [0,v,0]</td>
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<tr>
<td>8 c 2'm'..</td>
<td>0,1/4,1/4 [0,v,w]</td>
<td>0,3/4,1/4 [0,v,w]</td>
<td></td>
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<tr>
<td>4 b m'mm</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
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<tr>
<td>4 a m'mm</td>
<td>0,0,0 [0,0,0]</td>
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</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p2mm1'  
  \( \mathbf{a}^* = \mathbf{a}/2 \)  \( \mathbf{b}^* = \mathbf{b}/2 \)  
  Origin at 0,0,z  

- **Along [1,0,0]**: p2\( \mathbf{a}^* \)-2mm  
  \( \mathbf{a}^* = \mathbf{c}/2 \)  \( \mathbf{b}^* = \mathbf{b}/2 \)  
  Origin at x,0,0  

- **Along [0,1,0]**: p2mm1'  
  \( \mathbf{a}^* = \mathbf{c}/2 \)  \( \mathbf{b}^* = \mathbf{a}/2 \)  
  Origin at 0,y,0


**Symmetry Operations**

For $(0,0,0)$ + set

1. $1$
2. $2$ $0,0,z$
   
3. $2'$ $0,y,0$
   
4. $2'$ $x,0,0$

For $(0,1/2,1/2)$ + set

1. $t'$ $(0,1/2,1/2)$
2. $2'$ $(0,0,1/2) 0,1/4,z$
   
3. $2 (0,1/2,0) 0,y,1/4$
   
4. $2 (1/2,0,0) x,1/4,0$

For $(1/2,0,1/2)$ + set

1. $t$ $(1/2,0,1/2)$
2. $2' (0,0,1/2) 1/4,0,z$
   
3. $2 (1/2,0,0) 1/4,y,1/4$
   
4. $2 (1/2,0,0) x,0,1/4$

For $(1,2,0,1/2)$ + set

1. $t (1,2,0,1/2)$
2. $2' (0,0,1/2) 1/4,0,z$
   
3. $2 (1/2,0,0) 1/4,y,1/4$
   
4. $2 (1/2,0,0) x,0,1/4$

For $(1,2,1,2)$ + set

1. $t (1/2,1/2,0)$
2. $2 1/4,1/4,z$
   
3. $2' (0,1/2,0) 1/4,y,0$
   
4. $2' (1/2,0,0) x,1/4,0$

For $(1/2,1/2,0)$ + set

1. $t' (1/2,1/2,0)$
2. $2' (0,1/2,0) 1/4,y,0$
   
3. $2' (1/2,0,0) x,1/4,0$
   
4. $2' (1/2,0,0) x,1/4,0$

Origin at center (mmm')

Asymmetric unit

$0 \leq x \leq 1/4; 0 \leq y \leq 1/4; 0 \leq z \leq 1/2$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

Positions

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<td>(0,0,0) + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0) +</td>
<td>(0,0,0) + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0) +</td>
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<tr>
<td>32 p 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) x,y,z [u,v,w] (8) x,y,z [u,v,w]</td>
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<tr>
<td>8 h m2'm' 0,y,0 [u,0,0] 0,y,0 [u,0,0] 0,y,0 [u,0,0]</td>
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<tr>
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<td>8 d .2/m. 1/4,0,1/4 [0,v,0] 3/4,0,1/4 [0,v,0] 3/4,0,1/4 [0,v,0]</td>
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<tr>
<td>8 c 2/m.. 1/4,1/4 [u,0,0] 1/4,1/4 [u,0,0] 1/4,1/4 [u,0,0]</td>
<td>8 c 2/m.. 1/4,1/4 [u,0,0] 1/4,1/4 [u,0,0] 1/4,1/4 [u,0,0]</td>
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<td>4 a mmm' 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p_2/mmm
  \[
a^* = a/2 \quad b^* = b/2 \quad c^* = c/2
\]
  Origin at 0,0,z

- Along [1,0,0] p2mm1
  \[
a^* = b/2 \quad b^* = c/2 \quad a^* = c/2 \quad b^* = a/2
\]
  Origin at x,0,0

- Along [0,1,0] p2mm1
  \[
a^* = c/2 \quad b^* = a/2
\]
  Origin at 0,y,0
Orthorhombic

$$F_c m'm'm$$

$$mmm1'$$

$$F_c 2'/m'2'/m'2/m$$

Asymmetric unit:
$$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/2$$

Symmetry Operations:

For $$(0,0,0) +$$ set:

1. $$1$$
   $$(1 \mid 0,0,0)$$

2. $$2$$
   $$0,0,z$$
   $$(2_z \mid 0,0,0)$$

3. $$2'$$
   $$0,y,0$$
   $$(2_y \mid 0,0,0)'$$

4. $$2'$$
   $$x,0,0$$
   $$(2_x \mid 0,0,0)'$$

5. $$T$$
   $$0,0,0$$
   $$(T \mid 0,0,0)$$

6. $$m$$
   $$x,y,0$$
   $$(m_x \mid 0,0,0)$$

7. $$m'$$
   $$x,0,z$$
   $$(m_y \mid 0,0,0)'$$

8. $$m'$$
   $$0,y,z$$
   $$(m_z \mid 0,0,0)'$$

For $$(0,1/2,1/2)' +$$ set:

1. $$t'$$
   $$(0,1/2,1/2)$$
   $$(1 \mid 0,1/2,1/2)'$$

2. $$2'$$
   $$(0,0,1/2)$$
   $$0,1/4,z$$
   $$(2_z \mid 0,1/2,1/2)'$$

3. $$2$$
   $$(0,1/2,0)$$
   $$0,y,1/4$$
   $$(2_y \mid 0,1/2,1/2)$$

4. $$2$$
   $$x,1/4,1/4$$
   $$(2_x \mid 0,1/2,1/2)$$

5. $$T$$
   $$1/4,0,1/4$$
   $$(T \mid 1/2,0,1/2)$$

6. $$b'$$
   $$(0,1/2,0)$$
   $$x,y,1/4$$
   $$(m_x \mid 0,1/2,1/2)'$$

7. $$c$$
   $$(0,0,1/2)$$
   $$x,1/4,z$$
   $$(m_y \mid 0,1/2,1/2)$$

8. $$n$$
   $$(0,1/2,1/2)$$
   $$0,y,z$$
   $$(m_z \mid 0,1/2,1/2)'$$

For $$(1/2,0,1/2)' +$$ set:

1. $$t'$$
   $$(1/2,0,1/2)$$
   $$(1 \mid 1/2,0,1/2)'$$

2. $$2'$$
   $$(0,0,1/2)$$
   $$1/4,0,z$$
   $$(2_z \mid 1/2,0,1/2)'$$

3. $$2$$
   $$1/4,y,1/4$$
   $$(2_y \mid 1/2,0,1/2)$$

4. $$2$$
   $$(1/2,0,0)$$
   $$x,0,1/4$$
   $$(2_x \mid 1/2,0,1/2)'$$

5. $$T$$
   $$1/4,0,1/4$$
   $$(T \mid 1/2,0,1/2)'$$

6. $$a'$$
   $$(1/2,0,0)$$
   $$x,y,1/4$$
   $$(m_x \mid 1/2,0,1/2)'$$

7. $$n$$
   $$(1/2,0,1/2)$$
   $$x,0,z$$
   $$(m_y \mid 1/2,0,1/2)$$

8. $$c$$
   $$(0,0,1/2)$$
   $$1/4,y,z$$
   $$(m_z \mid 1/2,0,1/2)'$$

For $$(1/2,1,2,0) +$$ set:

1. $$t$$
   $$(1/2,1,2,0)$$
   $$(1 \mid 1/2,1,2,0)$$

2. $$2$$
   $$1/4,1/4,z$$
   $$(2_z \mid 1/2,1,2,0)$$

3. $$2'$$
   $$(0,1/2,0)$$
   $$1/4,y,0$$
   $$(2_y \mid 1/2,1,2,0)'$$

4. $$2'$$
   $$(1/2,0,0)$$
   $$x,1/4,0$$
   $$(2_x \mid 1/2,1,2,0)'$$

5. $$T$$
   $$1/4,1/4,0$$
   $$(T \mid 1/2,1,2,0)$$

6. $$n$$
   $$(1/2,1,2,0)$$
   $$x,y,0$$
   $$(m_x \mid 1/2,1,2,0)$$

7. $$a'$$
   $$(1/2,0,0)$$
   $$x,1/4,z$$
   $$(m_y \mid 1/2,1,2,0)'$$

8. $$b'$$
   $$(0,1/2,0)$$
   $$1/4,y,z$$
   $$(m_z \mid 1/2,1,2,0)'$$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>32 p 1</td>
<td>(0,0,0) + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0) +</td>
<td>x,y,z [u,v,w]</td>
<td>p2mm1'</td>
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<tr>
<td>16 o .m</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
<td>p2mm1'</td>
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<tr>
<td>16 n .m'</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>16 m m'..</td>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
<td>p2mm1'</td>
</tr>
<tr>
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<td>x,3/4,1/4 [u,0,0]</td>
<td>p2mm1'</td>
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<tr>
<td>16 k .2.</td>
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<td>3/4,y,1/4 [0,v,0]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>16 j .2</td>
<td>1/4,1/4,z [0,0,w]</td>
<td>3/4,1/4,z [0,0,w]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>8 i m'm'2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>8 h m'2'm</td>
<td>0,y,0 [0,0,w]</td>
<td>0,y,0 [0,0,w]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>8 g 2'm'm</td>
<td>x,0,0 [0,0,w]</td>
<td>x,0,0 [0,0,w]</td>
<td>p2mm1'</td>
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<tr>
<td>8 f 222</td>
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<td>3/4,3/4,3/4 [0,0,0]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>8 e .2/m</td>
<td>1/4,1/4,0 [0,0,w]</td>
<td>3/4,1/4,0 [0,0,w]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>8 d .2/m'</td>
<td>1/4,0,1/4 [0,0,0]</td>
<td>3/4,0,1/4 [0,0,0]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>8 c 2/m'..</td>
<td>0,1/4,1/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
<td>p2mm1'</td>
</tr>
<tr>
<td>4 b m'm'm</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
<td>p2mm1'</td>
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<tr>
<td>4 a m'm'm</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
<td>p2mm1'</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p2mm1' a* = a/2 b* = b/2 Origin at 0,0,z
- Along [1,0,0] p2mm1' a* = c/2 b* = b/2 Origin at x,0,1/4
- Along [0,1,0] p2mm1' a* = c/2 b* = a/2 Origin at 0,y,1/4
Asymmetric unit: 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set:

(1) 1
(1 0,0,0)
(5) T 0,0,0
(5 0,0,0)

For (0,1/2,1/2) + set:

(1) t' (0,1/2,1/2)
(1 0,1/2,1/2)
(5) T' 0,1/2,1/4
(5 0,1/2,1/2)

For (1/2,0,1/2) + set:

(1) t' (1/2,0,1/2)
(1 1/2,0,1/2)
(5) T' 1/4,0,1/4
(5 1/2,0,1/2)

For (1/2,1,2,0) + set:

(1) t (1/2,1/2,0)
(1 1/2,1/2,0)
(5) T' 1,4,1/4,0
(5 1/2,1/2,0)

### Orthorhombic

69.10.614

### mm'm'1'

69.10.614 Fc 2/m2'/m'2'/m'

### Origin

At center (mm'm')
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(0,1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

Positions

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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(0,1/2,1/2)' +</td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(1/2,0,1/2)' +</td>
<td>(3) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(1/2,1/2,0) +</td>
<td>(4) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>32 p 1</td>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

Coordinates

<table>
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<tr>
<th>(0,0,0) +</th>
<th>(0,1/2,1/2)' +</th>
<th>(1/2,0,1/2)' +</th>
<th>(1/2,1/2,0) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 16 o .m'     | x,y,0 [u,v,0]  | x,y,0 [u,v,0]  | x,y,0 [u,v,0] |
| 16 n .n'     | x,0,z [u,0,w]  | x,0,z [u,0,w]  | x,0,z [u,0,w] |
| 16 m n..     | 0,y,z [u,0,0]  | 0,y,z [u,0,0]  | 0,y,z [u,0,0] |
| 16 l 2'..    | x,1/4,1/4 [0,v,w] | x,1/4,1/4 [0,v,w] | x,1/4,1/4 [0,v,w] |
| 16 k .2.     | 1/4,y,1/4 [0,v,0] | 1/4,y,1/4 [0,v,0] | 1/4,y,1/4 [0,v,0] |
| 16 j .2'     | 1/4,1/4,z [u,0,v,0] | 1/4,1/4,z [u,0,v,0] | 1/4,1/4,z [u,0,v,0] |

Symmetry of Special Projections

Along [0,0,1] p_{c}, 2mm
\( a^* = a/2 \) \( b^* = b/2 \)
Origin at 0,1/4,z

Along [1,0,0] p_{2mm1'}
\( a^* = b/2 \) \( b^* = c/2 \)
Origin at x,0,0

Along [0,1,0] p_{2x}, 2mm
\( a^* = c/2 \) \( b^* = a/2 \)
Origin at 0,y,1/4

69.10.614 - 2 - 1220
**Symmetry Operations**

**For (0,0,0) + set**

1. \( \overline{1} \)
   - \((1|0,0,0)\)
   - \((2|0,0,z)\)
   - \((3|0,y,0)\)
   - \((4|x,0,0)\)

2. \( \overline{1} \)
   - \((0,1/2,1/2)\)
   - \((0,0,0)\)
   - \((0,1/2,1/2)\)
   - \((0,0,0)\)

3. \( \overline{1} \)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)

4. \( \overline{1} \)
   - \((1,0,0)\)
   - \((0,1/2,0)\)
   - \((1,0,0)\)
   - \((0,1/2,0)\)

5. \( \overline{1} \)
   - \((0,0,0)\)
   - \((0,0,0)\)
   - \((0,0,0)\)
   - \((0,0,0)\)

6. \( \overline{1} \)
   - \((0,1/2,0)\)
   - \((0,1/2,0)\)
   - \((0,1/2,0)\)
   - \((0,1/2,0)\)

7. \( \overline{1} \)
   - \((1/2,0,0)\)
   - \((1/2,0,0)\)
   - \((1/2,0,0)\)
   - \((1/2,0,0)\)

8. \( \overline{1} \)
   - \((1/2,0,0)\)
   - \((1/2,0,0)\)
   - \((1/2,0,0)\)
   - \((1/2,0,0)\)

**For (0,1/2,1/2) + set**

1. \( t \)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)

2. \( t \)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)

3. \( t \)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)

4. \( t \)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)

5. \( t \)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)

6. \( t \)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)

7. \( t \)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)

8. \( t \)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)

**For (1/2,0,1/2) + set**

1. \( a \)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)

2. \( a \)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)

3. \( a \)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)

4. \( a \)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)

5. \( a \)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)

6. \( a \)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)

7. \( a \)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)

8. \( a \)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)

**For (1/2,1/2,0) + set**

1. \( n \)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)

2. \( n \)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)

3. \( n \)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)

4. \( n \)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)

5. \( n \)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)
   - \((1/2,0,0)\)
   - \((0,1/2,0)\)

6. \( n \)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)
   - \((1/2,1/2,0)\)
   - \((0,1/2,1/2)\)

7. \( n \)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,0)\)

8. \( n \)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,0,1/2)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2); t'(1/2,0,1/2); (2); (3); (5).

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<td>(1/2,0,1/2)’+</td>
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<td>x,y,z [u,v,w]</td>
<td>32 p 1</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>32 p 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 o .m'</td>
<td>x,y,0 [u,v,0]</td>
<td>16 o .m'</td>
</tr>
<tr>
<td>16 n .m'</td>
<td>x,0,z [0,0,w]</td>
<td>16 n .m'</td>
</tr>
<tr>
<td>16 m .m'</td>
<td>0,y,z [0,0,w]</td>
<td>16 m .m'</td>
</tr>
<tr>
<td>16 l .m'</td>
<td>x,1/4,1/4 [0,0,w]</td>
<td>16 l .m'</td>
</tr>
<tr>
<td>16 k .m'</td>
<td>1/4,1/4,1/4 [u,0,w]</td>
<td>16 k .m'</td>
</tr>
<tr>
<td>16 j .m'</td>
<td>1/4,1/4,1/4 [0,0,w]</td>
<td>16 j .m'</td>
</tr>
<tr>
<td>8 i m'm'2</td>
<td>0,0,z [0,0,0]</td>
<td>8 i m'm'2</td>
</tr>
<tr>
<td>8 h m'm'</td>
<td>0,y,0 [0,0,0]</td>
<td>8 h m'm'</td>
</tr>
<tr>
<td>8 g 2m'm'</td>
<td>x,0,0 [u,0,0]</td>
<td>8 g 2m'm'</td>
</tr>
<tr>
<td>8 f 2'2'2</td>
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<td>8 f 2'2'2</td>
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<tr>
<td>8 e .m'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>8 e .m'</td>
</tr>
<tr>
<td>8 d .m'</td>
<td>1/4,0,1/4 [0,0,0]</td>
<td>8 d .m'</td>
</tr>
<tr>
<td>8 c 2'm'm'..</td>
<td>0,1/4,1/4 [u,0,0]</td>
<td>8 c 2'm'm'..</td>
</tr>
<tr>
<td>4 b m'm'm'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>4 b m'm'm'</td>
</tr>
<tr>
<td>4 a m'm'm'</td>
<td>0,0,0 [0,0,0]</td>
<td>4 a m'm'm'</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_c 2mm</th>
<th>Along [1,0,0]</th>
<th>p_{2a^*} 2m'm'</th>
<th>Along [0,1,0]</th>
<th>p_{2a^*} 2m'm'</th>
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<tbody>
<tr>
<td>a* = a/2</td>
<td>b* = b/2</td>
<td>a* = -c/2</td>
<td>b* = b/2</td>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 1/4,1/4,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Fdd mmm Orthorhombic**

70.1.616

**F2/d2/d2/d**

**Origin**

at 222 at -1/8,-1/8,-1/8 from \( \bar{1} \)

**Asymmetric unit**

\( 0 < x < 1/8; \quad 0 < y < 1/4; \quad 0 < z < 1 \)

**Symmetry Operations**

**For (0,0,0) + set**

1. \( \bar{1} \)  
2. \( (1\bar{0},0,0) \)
3. \( (2\bar{z},0,0,0) \)
4. \( x,0,0 \)
5. \( \bar{1}/8,1/8,1/8 \)
6. \( (1/4,1/4,0) x,y,1/8 \)
7. \( (1/4,0,1/4) x,1/8,z \)
8. \( (0,1/4,1/4) 1/8,y,z \)

**For (0,1/2,1/2) + set**

1. \( t (0,1/2,1/2) \)  
2. \( (1\bar{0},1/2,1/2) \)
3. \( (2\bar{z},0,1/2,1/2) \)
4. \( x,1/4,1/4 \)
5. \( \bar{1}/8,3/8,3/8 \)
6. \( (1/4,3/4,0) x,y,3/8 \)
7. \( (1/4,0,3/4) x,3/8,z \)
8. \( (0,3/4,3/4) 1/8,y,z \)

**For (1/2,0,1/2) + set**

1. \( t (1/2,0,1/2) \)  
2. \( (1\bar{0},0,1/2) \)
3. \( (2\bar{z},1/2,0,1/2) \)
4. \( x,0,1/4 \)
5. \( \bar{3}/8,1/8,3/8 \)
6. \( (3/4,1,4,0) x,y,3/8 \)
7. \( (3/4,0,3/4) x,1/8,z \)
8. \( (0,1/4,3/4) 3/8,y,z \)

**For (1/2,1/2,0) + set**

1. \( t (1/2,1/2,0) \)  
2. \( (1\bar{0},1/2,0) \)
3. \( (2\bar{z},1/2,1/2,0) \)
4. \( x,1/4,0 \)
5. \( \bar{3}/8,3/8,1/8 \)
6. \( (3/4,3,4,0) x,y,1/8 \)
7. \( (3/4,0,1/4) x,3/8,z \)
8. \( (0,3/4,1/4) 3/8,y,z \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
</tr>
<tr>
<td>32</td>
<td>h 1</td>
</tr>
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<td>16</td>
<td>g ..2</td>
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<td>16</td>
<td>f .2</td>
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<td>16</td>
<td>e 2..</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>d 1/8,1/8,1/8 [u,v,w]</td>
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<tr>
<td>8</td>
<td>b 222</td>
</tr>
<tr>
<td></td>
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</tr>
<tr>
<td>8</td>
<td>a 222</td>
</tr>
<tr>
<td></td>
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</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c_p 2m' m'  
Along [1,0,0]  c_p 2m' m'  
Along [0,1,0]  c_p 2m' m'  

a* = a/2  b* = b/2  
Origin at 0,0,z  

a* = b/2  b* = c/2  
Origin at x,0,0  

a* = c/2  b* = a/2  
Origin at 0,y,0
Origin at 22'' at -1/8,-1/8,-1/8 from 1''

Asymmetric unit $0 \leq x < 1/8$; $0 \leq y < 1/4$; $0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0) + \text{set}$

$(1) \text{ t (0,0,0)}$

$(2) \text{ 2 (0,0,z)}$

$(3) \text{ 2 (0,y,0)}$

$(4) \text{ 2 (x,0,0)}$

$(5) \text{ 1/8,1/8,z}$

$(6) \text{ d (1/4,1/4,0) x,y,1/8}$

$(7) \text{ d (1/4,0,1/4) x,1/8,z}$

$(8) \text{ d (0,1/4,1/4) 1/8,y,z}$

For $(0,1/2,1/2) + \text{set}$

$(1) \text{ t (0,1/2,1/2)}$

$(2) \text{ 2 (0,0,1/2) 0,1/4,z}$

$(3) \text{ 2 (0,1/2,0) 0,y,1/4}$

$(4) \text{ 2 (x,1/4,1/4)}$

$(5) \text{ 1/4,3/4,3/4}$

$(6) \text{ d (1/4,3/4,0) x,y,3/8}$

$(7) \text{ d (1/4,0,1/4) x,3/8,z}$

$(8) \text{ d (0,3/4,3/4) 1/8,y,z}$

For $(1/2,0,1/2) + \text{set}$

$(1) \text{ t (1/2,0,1/2)}$

$(2) \text{ 2 (0,0,1/2) 1/4,0,z}$

$(3) \text{ 2 (1/2,0,1/2) 1/4,y,1/4}$

$(4) \text{ 2 (1/2,0,0) x,0,1/4}$

$(5) \text{ 3/4,1/4,3/4}$

$(6) \text{ d (3/4,1/4,0) x,y,3/8}$

$(7) \text{ d (3/4,0,3/4) x,1/8,z}$

$(8) \text{ d (0,1/4,3/4) 3/8,y,z}$

For $(1/2,1/2,0) + \text{set}$

$(1) \text{ t (1/2,1/2,0)}$

$(2) \text{ 2 (1/2,1/2,0) 1/4,1/4,z}$

$(3) \text{ 2 (0,1/2,0) 1/4,y,0}$

$(4) \text{ 2 (1/2,0,0) x,1/4,0}$

$(5) \text{ 3/4,3/4,1/4}$

$(6) \text{ d (3/4,3/4,0) x,y,1/8}$

$(7) \text{ d (3/4,0,1/4) x,3/8,z}$

$(8) \text{ d (0,3/4,1/4) 3/8,y,z}$

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For (0,0,0)’ + set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(1) t’ (0,0,0)’</td>
<td>(0,0,0,z) [0,0,0]</td>
</tr>
<tr>
<td>(2) 2’ (0,0,0)’</td>
<td>(0,y,0) [0,0,0]</td>
</tr>
<tr>
<td>(3) 2’ (0,0,0)’</td>
<td>(x,0,0) [0,0,0]</td>
</tr>
<tr>
<td>(4) 2’ (0,0,0)’</td>
<td>(2,0,0) [0,0,0]</td>
</tr>
<tr>
<td>(5) T’ 1/8,1/8,1/8</td>
<td>(d’ (1/4,1/4,0) x,y,1/8)</td>
</tr>
<tr>
<td>(T</td>
<td>1/4,1/4,1/4)’</td>
</tr>
</tbody>
</table>

For (0,1/2,1/2)’ + set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t’ (0,1/2,1/2)’</td>
<td>(0,0,1/2,1/2)</td>
</tr>
<tr>
<td>(2) 2’ (0,0,1/2,1/2)’</td>
<td>(0,1/4,0,1/4)</td>
</tr>
<tr>
<td>(3) 2’ (0,1/2,0)</td>
<td>(0,1/4,0,1/4)</td>
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<tr>
<td>(4) 2’ (0,1/2,0)</td>
<td>(2,0,1/2,1/2)</td>
</tr>
<tr>
<td>(5) T’ 1/8,3/8,3/8</td>
<td>(d’ (1/4,3/4,0) x,y,3/8)</td>
</tr>
<tr>
<td>(T</td>
<td>1/4,3/4,3/4)’</td>
</tr>
</tbody>
</table>

For (1/2,0,1/2)’ + set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t’ (1/2,0,1/2)’</td>
<td>(0,0,1/2,1/2)</td>
</tr>
<tr>
<td>(2) 2’ (1/2,0,1/2)’</td>
<td>(1/4,0,1/4)</td>
</tr>
<tr>
<td>(3) 2’ (1/2,0,1/2)’</td>
<td>(1/4,0,1/4)</td>
</tr>
<tr>
<td>(4) 2’ (1/2,0,1/2)’</td>
<td>(2,1/2,1/2)</td>
</tr>
<tr>
<td>(5) T’ 3/8,1/8,3/8</td>
<td>(d’ (3/4,1/4,0) x,y,3/8)</td>
</tr>
<tr>
<td>(T</td>
<td>3/4,1/4,3/4)’</td>
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</tbody>
</table>

For (1/2,1/2,0)’ + set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t’ (1/2,1/2,0)’</td>
<td>(0,0,1/2,1/2)</td>
</tr>
<tr>
<td>(2) 2’ (1/2,1/2,0)’</td>
<td>(1/4,1/4,0)</td>
</tr>
<tr>
<td>(3) 2’ (1/2,1/2,0)’</td>
<td>(1/4,1/4,0)</td>
</tr>
<tr>
<td>(4) 2’ (1/2,1/2,0)’</td>
<td>(2,1/2,1/2)</td>
</tr>
<tr>
<td>(5) T’ 3/8,3/8,1/8</td>
<td>(d’ (3/4,3/4,0) x,y,1/8)</td>
</tr>
<tr>
<td>(T</td>
<td>3/4,3/4,1/4)’</td>
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</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); 1’.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>32 h 11'</td>
<td>(1) x,y,z [0,0,0]</td>
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</tr>
<tr>
<td></td>
<td>(2) x + 1/4, y + 1/4, z + 1/4 [0,0,0]</td>
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<tr>
<td></td>
<td>(3) x,y,z [0,0,0]</td>
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<td>(4) x,y,z [0,0,0]</td>
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<tr>
<td></td>
<td>(5) x,y,z [0,0,0]</td>
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<tr>
<td></td>
<td>(6) x + 1/4, y + 1/4, z + 1/4 [0,0,0]</td>
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</tr>
<tr>
<td></td>
<td>(7) x + 1/4, y + 1/4, z + 1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>16 g ..21'</td>
<td>(0,0,0) [0,0,0]</td>
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<td>(0,0,0) [0,0,0]</td>
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<td>(0,0,0) [0,0,0]</td>
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<td>(0,0,0) [0,0,0]</td>
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<tr>
<td>16 f ..21'</td>
<td>(0,0,0) [0,0,0]</td>
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<td>(0,0,0) [0,0,0]</td>
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<td>(0,0,0) [0,0,0]</td>
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</tbody>
</table>

70.2.617 - 2 - 1226
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>沿线</th>
<th>投影</th>
<th>原点</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[0,0,1]$</td>
<td>c2mm1'</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td>$[1,0,0]$</td>
<td>c2mm1'</td>
<td>$x,0,0$</td>
</tr>
<tr>
<td>$[0,0,0]$</td>
<td>c2mm1'</td>
<td>$0,y,0$</td>
</tr>
</tbody>
</table>

### Note

$a^* = a/2$  $b^* = b/2$  $c^* = c/2$
Origin at 22'2' at -1/8, -1/8, -1/8 from T'

Asymmetric unit 0 ≤ x ≤ 1/8; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) T (1 | 0,0,0)
(2) 2' 0,0,z (2 | 0,0,0)
(3) 2' 0,y,0 (2 | 0,0,0)
(4) 2 0,0,0 (2 | 0,0,0)
(5) T' 1/8,1/8,1/8 (1 | 1/4,1/4,1/4)
(6) d (1/4,1/4,0) x,y,1/8 (m_z | 1/4,1/4,1/4)
(7) d (1/4,0,1/4) x,1/8,z (m_y | 1/4,1/4,1/4)
(8) d' (0,1/4,1/4) 1/8,y,z (m_x | 1/4,1/4,1/4)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (1 | 0,1/2,1/2)
(2) 2' (0,0,1/2) 0,1/4,z (2 | 0,1/2,1/2)
(3) 2' (0,1/2,0) 0,y,1/4 (2 | 0,1/2,1/2)
(4) 2 x,1/4,1/4 (2 | 0,1/2,1/2)
(5) T' 1/8,3/8,3/8 (1 | 1/4,3/4,3/4)
(6) d (1/4,3/4,0) x,y,3/8 (m_z | 1/4,3/4,3/4)
(7) d (1/4,0,1/4) x,3/8,z (m_y | 1/4,3/4,3/4)
(8) d' (0,3/4,1/4) 3/8,y,z (m_x | 1/4,3/4,3/4)

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2) (1 | 1/2,0,1/2)
(2) 2' (0,0,1/2) 1/4,0,z (2 | 1/2,0,1/2)
(3) 2' 1/4,y,1/4 (2 | 1/2,0,1/2)
(4) 2 x,0,1/4 (2 | 1/2,0,1/2)
(6) d (3/4,1/4,0) x,y,3/8 (m_z | 3/4,1/4,3/4)
(7) d (3/4,0,3/4) x,1/8,z (m_y | 3/4,1/4,3/4)
(8) d' (0,1/4,3/4) 3/8,y,z (m_x | 3/4,1/4,3/4)

For (1/2,1,2,0) + set

(1) t (1/2,1/2,0) (1 | 1/2,1/2,0)
(2) 2' 1/4,1/4,z (2 | 1/2,1/2,0)
(3) 2' (0,1/2,0) 1/4,y,0 (2 | 1/2,1/2,0)
(4) 2 x,1/4,0 (2 | 1/2,1/2,0)
(6) d (3/4,3/4,0) x,y,1/8 (m_z | 3/4,3/4,1/4)
(7) d (3/4,0,1/4) x,3/8,z (m_y | 3/4,3/4,1/4)
(8) d' (0,3/4,1/4) 3/8,y,z (m_x | 3/4,3/4,1/4)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
</tr>
<tr>
<td>32 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) x̄,y,z [ū,v̄,w]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x+1/4,y+1/4,z+1/4 [ū,v̄,w]</td>
<td>(6) x+1/4,y+1/4,z+1/4 [u,v,w]</td>
</tr>
<tr>
<td>(7) x+1/4,y+1/4,z+1/4 [u,v,w]</td>
<td>(8) x̄+1/4,y+1/4,z+1/4 [ū,v̄,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c_p 2'mm'  
Along [1,0,0] c2mm  
Along [0,1,0] c_p 2'mm'

<table>
<thead>
<tr>
<th>a* = a/2</th>
<th>b* = b/2</th>
<th>c* = c/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>
Origin at 2'2'2 at -1/8, -1/8, -1/8 from $\overline{1}$

Asymmetric unit $0 \leq x \leq 1/8; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) $t$ $\quad$ (2) $2 \quad$ $0,0,z$ $\quad$ (3) $2' \quad$ $0,y,0$ $\quad$ (4) $2' \quad$ $x,0,0$

$\quad$ $\quad$ (2z $\quad$ $0,0,0$) $\quad$ (2z $\quad$ $0,0,0$) $\quad$ (2z $\quad$ $0,0,0$)$'$

(5) $\overline{1}$ $\quad$ 1/8, 1/8, 1/8 $\quad$ (6) $d \quad$ (1/4, 1/4, 0) $\quad$ x,y,1/8 $\quad$ (7) $d' \quad$ (1/4, 0, 1/4) $\quad$ x,1/8,z $\quad$ (8) $d' \quad$ (0, 1/4, 1/4) $\quad$ 1/8,y,z

$\quad$ (1/4, 1/4, 1/4) $\quad$ (1/4, 1/4, 1/4) $\quad$ (1/4, 1/4, 1/4)$'$

For (0,1/2,1/2) + set

(1) $t \quad$ (0,1/2,1/2) $\quad$ (2) $2 \quad$ (0,0,1/2) $\quad$ 0,1/4,z $\quad$ (3) $2' \quad$ (0,1/2,0) $\quad$ 0,y,1/4 $\quad$ (4) $2' \quad$ x,1/4,1/4

$\quad$ (1/2,1/2,1/2) $\quad$ (1/2,0,1/2) $\quad$ (1/2,0,1/2)$'$ $\quad$ (2z $\quad$ 0,1/2,1/2) $\quad$ (2z $\quad$ 0,1/2,1/2)$'$

(5) $\overline{1}$ $\quad$ 1/8, 3/8, 3/8 $\quad$ (6) $d \quad$ (1/4, 3/4, 0) $\quad$ x,y,3/8 $\quad$ (7) $d' \quad$ (1/4, 0, 3/4) $\quad$ x,3/8,z $\quad$ (8) $d' \quad$ (0, 3/4, 3/4) $\quad$ 1/8,y,z

$\quad$ (1/4, 3/4, 3/4) $\quad$ (1/4, 3/4, 3/4)$'$ $\quad$ (1/4, 3/4, 3/4)$'$

For (1/2,0,1/2) + set

(1) $t \quad$ (1/2,0,1/2) $\quad$ (2) $2 \quad$ (0,0,1/2) $\quad$ 1/4,0,z $\quad$ (3) $2' \quad$ 1/4, y,1/4 $\quad$ (4) $2' \quad$ x,1/4,0,1/4

$\quad$ (1/2,1/2,0) $\quad$ (1/2,0,1/2) $\quad$ (1/2,0,1/2)$'$ $\quad$ (2z $\quad$ 1/2,0,1/2) $\quad$ (2z $\quad$ 1/2,0,1/2)$'$

(5) $\overline{1}$ $\quad$ 3/8, 1/8, 3/8 $\quad$ (6) $d \quad$ (3/4, 1/4, 0) $\quad$ x,y,3/8 $\quad$ (7) $d' \quad$ (3/4, 0, 3/4) $\quad$ x,3/8,z $\quad$ (8) $d' \quad$ (0, 3/4, 3/4) $\quad$ 3/8,y,z

$\quad$ (3/4, 1/4, 3/4) $\quad$ (3/4, 1/4, 3/4)$'$ $\quad$ (3/4, 1/4, 3/4)$'$

For (1/2,1/2,0) + set

(1) $t \quad$ (1/2,1/2,0) $\quad$ (2) $2 \quad$ 1/4,1/4, z $\quad$ (3) $2' \quad$ (0,1/2,0) $\quad$ 1/4,y,0 $\quad$ (4) $2' \quad$ x,1/4,0

$\quad$ (1/2,1/2,0) $\quad$ (1/2,1/2,0) $\quad$ (1/2,1/2,0)$'$ $\quad$ (2z $\quad$ 1/2,1/2,0) $\quad$ (2z $\quad$ 1/2,1/2,0)$'$

(5) $\overline{1}$ $\quad$ 3/8, 3/8, 1/8 $\quad$ (6) $d \quad$ (3/4, 3/4, 0) $\quad$ x,y,1/8 $\quad$ (7) $d' \quad$ (3/4, 0, 1/4) $\quad$ x,3/8,z $\quad$ (8) $d' \quad$ (0, 3/4, 1/4) $\quad$ 3/8,y,z

$\quad$ (3/4, 3/4, 1/4) $\quad$ (3/4, 3/4, 1/4)$'$ $\quad$ (3/4, 3/4, 1/4)$'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td></td>
</tr>
</tbody>
</table>

32  h  1  
(1) x,y,z [u,v,w] 
(2) \(\bar{x}, \bar{y}, \bar{z} \) [\(\bar{u}, \bar{v}, \bar{w}\)] 
(3) \(x, y, z \) [u,v,w] 
(4) \(x, y, z \) [u,v,w] 
(5) \(x + 1/4, y + 1/4, z + 1/4 \) [u,v,w] 
(6) \(x + 1/4, y + 1/4, z + 1/4 \) [u,v,w] 
(7) \(x + 1/4, y + 1/4, z + 1/4 \) [u,v,w] 
(8) \(x + 1/4, y + 1/4, z + 1/4 \) [u,v,w]

16  g  .2  0,0,z [0,0,w]  0,0,\(\bar{z} \) [0,0,w]  1/4,1/4,\(\bar{z} + 1/4 \) [0,0,\(\bar{w}\)]  1/4,1/4,\(\bar{z} + 1/4 \) [0,0,\(\bar{w}\)]

16  f  .2'  0,y,0 [u,0,w]  0,y,0 [u,0,w]  1/4,\(y + 1/4, 1/4 \) [u,0,w]  1/4,\(y + 1/4, 1/4 \) [u,0,w]

16  e  2'..  x,0,0 [0,v,w]  \(\bar{x}, 0,0 \) [0,\(\bar{v}, \bar{w}\)]  \(\bar{x} + 1/4, 1/4, 1/4 \) [0,v,w]  \(x + 1/4, 1/4, 1/4 \) [0,\(\bar{v}, \bar{w}\)]

16  d  \(\bar{1} \)  5/8,5/8,5/8 [u,v,w]  3/8,3/8,5/8 [u,\(\bar{v}, \bar{w}\)]  3/8,5/8,3/8 [u,\(\bar{v}, \bar{w}\)]  5/8,3/8,3/8 [u,\(\bar{v}, \bar{w}\)]

16  c  \(\bar{1} \)  1/8,1/8,1/8 [u,v,w]  7/8,7/8,1/8 [u,\(\bar{v}, \bar{w}\)]  7/8,1/8,7/8 [u,\(\bar{v}, \bar{w}\)]  1/8,7/8,7/8 [u,\(\bar{v}, \bar{w}\)]

8  b  2'2'  0,0,1/2 [0,0,w]  1/4,1/4,3/4 [0,0,w]

8  a  2'2'  0,0,0 [0,0,w]  1/4,1/4,1/4 [0,0,w]

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c(\alpha), 2mm</th>
<th>Along [1,0,0]</th>
<th>c 2'mm'</th>
<th>Along [0,1,0]</th>
<th>c 2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a/2)</td>
<td>(b^* = b/2)</td>
<td>(a^* = -c/2)</td>
<td>(b^* = b/2)</td>
<td>(a^* = c/2)</td>
<td>(b^* = a/2)</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
Origin at 222 at -1/8, -1/8, -1/8 from \( \overline{1} \)

Asymmetric unit

\[
0 \leq x \leq 1/8; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1
\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1,0,0,0) \\
(5) & \quad \overline{1} \quad 1/8,1/8,1/8 \\
(5) & \quad (\overline{1} \quad 1/4,1/4,1/4)'
\end{align*}
\]

\[
\begin{align*}
(6) & \quad d' \quad (1/4,1/4,0) \quad x,y,1/8 \\
(6) & \quad (m_z \quad 1/4,1/4,1/4)'
\end{align*}
\]

\[
\begin{align*}
(7) & \quad d' \quad (1/4,0,1/4) \quad x,1/8,z \\
(7) & \quad (m_y \quad 1/4,1/4,1/4)'
\end{align*}
\]

\[
\begin{align*}
(8) & \quad d' \quad (0,1/4,1/4) \quad 1/8,y,z \\
(8) & \quad (m_\overline{1} \quad 1/4,1/4,1/4)'
\end{align*}
\]

For \((0,1/2,1/2) + \) set

\[
\begin{align*}
(1) & \quad t \quad (0,1/2,1/2) \\
(1) & \quad (1,0,1/2,1/2) \\
(5) & \quad \overline{1} \quad 1/8,3/8,3/8 \\
(5) & \quad (\overline{1} \quad 1/4,3/4,3/4)'
\end{align*}
\]

\[
\begin{align*}
(6) & \quad d' \quad (1/4,3/4,0) \quad x,y,3/8 \\
(6) & \quad (m_z \quad 1/4,3/4,3/4)'
\end{align*}
\]

\[
\begin{align*}
(7) & \quad d' \quad (1/4,0,1/4) \quad x,3/8,z \\
(7) & \quad (m_y \quad 1/4,3/4,3/4)'
\end{align*}
\]

\[
\begin{align*}
(8) & \quad d' \quad (0,3/4,3/4) \quad 1/8,y,z \\
(8) & \quad (m_\overline{1} \quad 1/4,3/4,3/4)'
\end{align*}
\]

For \((1/2,0,1/2) + \) set

\[
\begin{align*}
(1) & \quad t \quad (1/2,0,1/2) \\
(1) & \quad (1,2,0,1/2) \\
(5) & \quad \overline{1} \quad 3/8,1/8,3/8 \\
(5) & \quad (\overline{1} \quad 3/4,1/4,3/4)'
\end{align*}
\]

\[
\begin{align*}
(6) & \quad d' \quad (3/4,1/4,0) \quad x,y,3/8 \\
(6) & \quad (m_z \quad 3/4,1/4,3/4)'
\end{align*}
\]

\[
\begin{align*}
(7) & \quad d' \quad (3/4,0,3/4) \quad x,1/8,z \\
(7) & \quad (m_y \quad 3/4,1/4,3/4)'
\end{align*}
\]

\[
\begin{align*}
(8) & \quad d' \quad (0,1/4,3/4) \quad 3/8,y,z \\
(8) & \quad (m_\overline{1} \quad 3/4,1/4,3/4)'
\end{align*}
\]

For \((1/2,1,2,0) + \) set

\[
\begin{align*}
(1) & \quad t \quad (1/2,1,2,0) \\
(1) & \quad (1,2,1,2,0) \\
(5) & \quad \overline{1} \quad 3/8,3/8,1/8 \\
(5) & \quad (\overline{1} \quad 3/4,3/4,1/4)'
\end{align*}
\]

\[
\begin{align*}
(6) & \quad d' \quad (3/4,3/4,0) \quad x,y,1/8 \\
(6) & \quad (m_z \quad 3/4,3/4,1/4)'
\end{align*}
\]

\[
\begin{align*}
(7) & \quad d' \quad (3/4,0,1/4) \quad x,3/8,z \\
(7) & \quad (m_y \quad 3/4,3/4,1/4)'
\end{align*}
\]

\[
\begin{align*}
(8) & \quad d' \quad (0,3/4,1/4) \quad 3/8,y,z \\
(8) & \quad (m_\overline{1} \quad 3/4,3/4,1/4)'
\end{align*}
\]

70.5.620 - 1 - 1232
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
<td></td>
</tr>
</tbody>
</table>

| (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] |
| (3) x,y,z [u,v,w] | (4) x,y,z [u,v,w] |
| (5) x+1/4,y+1/4,z+1/4 [u,v,w] | (6) x+1/4,y+1/4,z+1/4 [u,v,w] |
| (7) x+1/4,y+1/4,z+1/4 [u,v,w] | (8) x+1/4,y+1/4,z+1/4 [u,v,w] |

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] c 2m'm' a&quot; = a/2 b&quot; = b/2</td>
</tr>
<tr>
<td>Along [1,0,0] c 2m'm' a&quot; = b/2 b&quot; = c/2</td>
</tr>
<tr>
<td>Along [0,1,0] c 2m'm' a&quot; = c/2 b&quot; = a/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z Origin at 0,0,z Origin at x,0,0
Immm | mmm | Orthorhombic
71.1.621 | I2/m2/m2/m

Origin at center (mmm)

Asymmetric unit
$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) +$ set

(1) $1$
$\begin{array}{c}
(1) 0,0,0
\end{array}$

(2) $2 \begin{array}{c}
0,0,z
(2_{z} 0,0,0)
\end{array}$

(3) $2 \begin{array}{c}
y,0,0
(2_{y} 0,0,0)
\end{array}$

(4) $2 \begin{array}{c}
x,0,0
(2_{x} 0,0,0)
\end{array}$

(5) $\bar{1} \begin{array}{c}
0,0,0
\end{array}$

(6) $m \begin{array}{c}
x,y,0
(m_{z} 0,0,0)
\end{array}$

(7) $m \begin{array}{c}
x,0,z
(m_{y} 0,0,0)
\end{array}$

(8) $m \begin{array}{c}
y,0,z
(m_{x} 0,0,0)
\end{array}$

For $(1/2,1/2,1/2) +$ set

(1) $t \begin{array}{c}
(1/2,1/2,1/2)
\end{array}$

(2) $2 \begin{array}{c}
(0,0,1/2)
(2_{z} 1/2,1/2,1/2)
\end{array}$

(3) $2 \begin{array}{c}
(0,1/2,0)
(2_{y} 1/2,1/2,1/2)
\end{array}$

(4) $2 \begin{array}{c}
(1/2,0,0)
(2_{x} 1/2,1/2,1/2)
\end{array}$

(5) $\bar{1} \begin{array}{c}
(1/2,1/2,1/2)
\end{array}$

(6) $n \begin{array}{c}
(1/2,1/2,0)
(m_{z} 1/2,1/2,1/2)
\end{array}$

(7) $n \begin{array}{c}
(1/2,0,1/2)
(m_{y} 1/2,1/2,1/2)
\end{array}$

(8) $n \begin{array}{c}
(0,1/2,1/2)
(m_{x} 1/2,1/2,1/2)
\end{array}$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x ,y ,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x ,y ,z [u,v,w]</td>
</tr>
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<td>(4) x ,y ,z [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x ,y ,z [u,v,w]</td>
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<tr>
<td></td>
<td>(6) x ,y ,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x ,y ,z [u,v,w]</td>
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<tr>
<td></td>
<td>(8) x ,y ,z [u,v,w]</td>
</tr>
<tr>
<td>8 n .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x ,y ,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x ,y ,0 [0,0,w]</td>
</tr>
<tr>
<td>8 m .m.</td>
<td>x,0,z [0,v,0]</td>
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<td>x ,0 ,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>x ,0 ,z [0,v,0]</td>
</tr>
<tr>
<td>8 l m..</td>
<td>0,y,z [u,0,0]</td>
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<tr>
<td></td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [u,0,0]</td>
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<tr>
<td>8 k I</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
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<tr>
<td>4 j mm2</td>
<td>1/2,0,z [0,0,0]</td>
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<td>1/2,0,z [0,0,0]</td>
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<tr>
<td>4 i mm2</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 h mm2m</td>
<td>0,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 g mm2m</td>
<td>0,y,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,0 [0,0,0]</td>
</tr>
<tr>
<td>4 f 2mm</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x ,1/2,0 [0,0,0]</td>
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<tr>
<td>4 e 2mm</td>
<td>x,0,0 [0,0,0]</td>
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<tr>
<td></td>
<td>x ,0 ,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d mmm</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c mmm</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b mmm</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a mmm</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1' 
\(a^* = a \quad b^* = b\)
Origin at 0,0,z

Along [1,0,0] c2mm1' 
\(a^* = b \quad b^* = c\)
Origin at x,0,0

Along [0,1,0] c2mm1' 
\(a^* = c \quad b^* = a\)
Origin at 0,y,0
Immm1'  
71.2.622  

Orthorhombic  

m1m1'  
I2/m2/m2/m1'  

Origin at center (mmm1')  
Asymmetric unit  
0 < x < 1/4; 0 < y < 1/2; 0 < z < 1/2  

Symmetry Operations  

For (0,0,0) + set  

(1) 1  
(1 0,0,0)  

(2) 2  0,0,z  
(2z 0,0,0)  

(3) 2  0,y,0  
(2y 0,0,0)  

(4) 2  x,0,0  
(2x 0,0,0)  

(5) T  0,0,0  
(T 0,0,0)  

(6) m  x,y,0  
(mz 0,0,0)  

(7) m  x,0,z  
(my 0,0,0)  

(8) m  0,y,z  
(m 0,0,0)  

For (1/2,1/2,1/2) + set  

(1) t (1/2,1/2,1/2)  
(1 1/2,1/2,1/2)  

(2) 2 (0,0,1/2)  1/4,1/4,z  
(2z 1/2,1/2,1/2)  

(3) 2 (0,1/2,0)  1/4,y,1/4  
(2y 1/2,1/2,1/2)  

(4) 2 (1/2,0,0)  x,1/4,1/4  
(2x 1/2,1/2,1/2)  

(5) T'  1/4,1/4,1/4  
(T' 1/2,1/2,1/2)  

(6) n (1/2,1/2,0)  x,y,1/4  
(mz 1/2,1/2,1/2)  

(7) n (1/2,0,1/2)  x,1/4,z  
(my 1/2,1/2,1/2)  

(8) n (0,1/2,1/2)  1/4,y,z  
(m 1/2,1/2,1/2)  

For (0,0,0)' + set  

(1) 1'  
(1 0,0,0)'  

(2) 2'  0,0,z  
(2z' 0,0,0)'  

(3) 2'  0,y,0  
(2y' 0,0,0)'  

(4) 2'  x,0,0  
(2x' 0,0,0)'  

(5) T'  0,0,0  
(T' 0,0,0)'  

(6) m'  x,y,0  
(mz' 0,0,0)'  

(7) m'  x,0,z  
(my' 0,0,0)'  

(8) m'  0,y,z  
(m' 0,0,0)'  

For (1/2,1/2,1/2)' + set  

(1) t' (1/2,1/2,1/2)  
(1 1/2,1/2,1/2)'  

(2) 2' (0,0,1/2)  1/4,1/4,z  
(2z 1/2,1/2,1/2)'  

(3) 2' (0,1/2,0)  1/4,y,1/4  
(2y 1/2,1/2,1/2)'  

(4) 2' (1/2,0,0)  x,1/4,1/4  
(2x 1/2,1/2,1/2)'  

(5) T'  1/4,1/4,1/4  
(T' 1/2,1/2,1/2)'  

(6) n' (1/2,1/2,0)  x,y,1/4  
(mz 1/2,1/2,1/2)'  

(7) n' (1/2,0,1/2)  x,1/4,z  
(my 1/2,1/2,1/2)'  

(8) n' (0,1/2,1/2)  1/4,y,z  
(m 1/2,1/2,1/2)'  

71.2.622 - 1 - 1236
### Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,0)' + (1/2,1/2,1/2) + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
<tr>
<td>16 o 11'</td>
<td>(1) x,y,z [0,0,0] (2) x , y , z [0,0,0] (3) x , y , z [0,0,0] (4) x , y , z [0,0,0] (5) x , y , z [0,0,0] (6) x , y , z [0,0,0] (7) x , y , z [0,0,0] (8) x , y , z [0,0,0]</td>
</tr>
<tr>
<td>8 n .m1'</td>
<td>x , y , 0 [0,0,0] x , y , 0 [0,0,0] x , y , 0 [0,0,0] x , y , 0 [0,0,0]</td>
</tr>
<tr>
<td>8 m .m1'</td>
<td>x , 0 , z [0,0,0] x , 0 , z [0,0,0] x , 0 , z [0,0,0] x , 0 , z [0,0,0]</td>
</tr>
<tr>
<td>8 l m..1'</td>
<td>0 , y , z [0,0,0] 0 , y , z [0,0,0] 0 , y , z [0,0,0] 0 , y , z [0,0,0]</td>
</tr>
<tr>
<td>8 k 1/1'</td>
<td>1/4 , 1/4 , 1/4 [0,0,0] 3/4 , 3/4 , 1/4 [0,0,0] 3/4 , 1/4 , 3/4 [0,0,0] 1/4 , 3/4 , 3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 j mm21'</td>
<td>1/2 , 0 , z [0,0,0] 1/2 , 0 , z [0,0,0]</td>
</tr>
<tr>
<td>4 i mm21'</td>
<td>0 , 0 , z [0,0,0] 0 , 0 , z [0,0,0]</td>
</tr>
<tr>
<td>4 h m2m1'</td>
<td>0 , y , 1/2 [0,0,0] 0 , y , 1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 g m2m1'</td>
<td>0 , y , 0 [0,0,0] 0 , y , 0 [0,0,0]</td>
</tr>
<tr>
<td>4 f 2mm1'</td>
<td>x , 1/2 , 0 [0,0,0] x , 1/2 , 0 [0,0,0]</td>
</tr>
<tr>
<td>4 e 2mm1'</td>
<td>x , 0 , 0 [0,0,0] x , 0 , 0 [0,0,0]</td>
</tr>
<tr>
<td>2 d mmm1'</td>
<td>1/2 , 0 , 1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c mmm1'</td>
<td>1/2 , 1/2 , 0 [0,0,0]</td>
</tr>
<tr>
<td>2 b mmm1'</td>
<td>0 , 1/2 , 1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a mmm1'</td>
<td>0 , 0 , 0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = a</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Im'mm  
71.3.623

m'mm  
l2/m'2'/m2'/m

Orthorhombic

Origin at center (m'mm)

Asymmetric unit  
0 < x < 1/4;  0 < y < 1/2;  0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

(1)  
(1 0,0,0)

(5)  
(1 0,0,0)

(1)  
(1 1/2,1/2,1/2)

(2) 2'  0,0,z  
(2z 0,0,0')

(6) m  x,y,0  
(mz 0,0,0)

(3) 2'  0,y,0  
(2y 0,0,0')

(7) m  x,0,z  
(my 0,0,0)

(4) 2  x,0,0  
(2x 0,0,0)

(8) m'  0,y,z  
(mz 0,0,0')

For (1/2,1/2,1/2) + set

(1) t  (1/2,1/2,1/2)

(2) 2'  (0,0,1/2)  
(2z 1/2,1/2,1/2')

(6) n  (1/2,1/2,0)  
(mz 1/2,1/2,1/2)

(3) 2'  (0,1/2,0)  
(2y 1/2,1/2,1/2')

(7) n  (1/2,0,1/2)  
(my 1/2,1/2,1/2)

(4) 2  (1/2,0,0)  
(2x 1/2,1/2,1/2)

(8) n'  (0,1/2,1/2)  
(mx 1/2,1/2,1/2')

71.3.623 - 1 - 1238
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
<td>(6) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
</tr>
<tr>
<td>8 n..m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 m..m'</td>
<td>x̅,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 l m'..</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 k 1</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 j m'm2'</td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 i m'm2'</td>
<td>0,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 h m'2'm</td>
<td>0,y,1/2 [0,w,0]</td>
</tr>
<tr>
<td>4 g m'2'm</td>
<td>0,y,0 [0,w,0]</td>
</tr>
<tr>
<td>4 f 2mm</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 e 2mm</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d m'2m</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c m'2m</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b m'2m</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a m'2m</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
<th>Along [1,0,0]</th>
<th>c2mm</th>
<th>Along [0,1,0]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = c</td>
<td>b* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at 0,y,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Im"m"m
71.4.624

m"m"m
l2'/m'2'/m'2/m

Orthorhombic

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2 | 0,0,0)

(3) 2' 0,y,0
(2' | 0,0,0')

(4) 2' x,0,0
(2 | 0,0,0)

(5) T 0,0,0
(T | 0,0,0)

(6) m x,y,0
(m | 0,0,0)

(7) m' x,0,z
(m' | 0,0,0')

(8) m' 0,y,z
(m' | 0,0,0')

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2 | 1/2,1/2,1/2)

(3) 2' (0,1/2,0) 1/4,y,1/4
(2' | 1/2,1/2,1/2')

(4) 2' (1/2,0,0) x,1/4,1/4
(2 | 1/2,1/2,1/2')

(5) T 1/4,1/4,1/4
(T | 1/2,1/2,1/2)

(6) n (1/2,1/2,0) x,y,1/4
(m | 1/2,1/2,1/2)

(7) n' (1/2,0,1/2) x,1/4,z
(m' | 1/2,1/2,1/2')

(8) n' (0,1/2,1/2) 1/4,y,z
(m' | 1/2,1/2,1/2')
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) x,y,z [u,v,w] (8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 n.m</td>
<td>x,y,0 [0,0,w] x,y,0 [0,0,w] x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 m.m'</td>
<td>x,0,z [u,0,w] x,0,z [u,0,w] x,0,z [u,0,w]</td>
</tr>
<tr>
<td>8 l.m'</td>
<td>0,y,z [0,v,w] 0,y,z [0,v,w] 0,y,z [0,v,w]</td>
</tr>
<tr>
<td>4 j m'm'2</td>
<td>1/2,0,z [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 i m'm'2</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 h m'2m</td>
<td>0,y,1/2 [0,0,w] 0,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 g m'2m</td>
<td>0,y,0 [0,0,w] 0,y,0 [0,0,w]</td>
</tr>
<tr>
<td>4 f 2'm'm</td>
<td>x,1/2,0 [0,0,w] x,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 e 2'm'm</td>
<td>x,0,0 [0,0,w] x,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2 d m'm'm</td>
<td>1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c m'm'm</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 b m'm'm</td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a m'm'm</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,0,0] c2'mm' Along [0,1,0] c2'mm'

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z \[ a^* = -c \quad b^* = b \]

Origin at x,0,0 \[ a^* = c \quad b^* = a \]

Origin at 0,y,0
Im'm'm'  
71.5.625  
Orthorhombic

m'm'm'  
l2/m'2/m'2/m'

Origin at center (m'm'm')

Asymmetric unit  
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) \( \begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix} \)

(2) \( \begin{pmatrix} 2 \\ 0,0,0 \end{pmatrix} \)

(3) \( \begin{pmatrix} 2 \\ 0,y,0 \end{pmatrix} \)

(4) \( \begin{pmatrix} 2 \\ x,0,0 \end{pmatrix} \)

(5) \( \begin{pmatrix} \bar{1} \\ 0,0,0 \end{pmatrix} \)

(6) \( \begin{pmatrix} m' \\ x,y,0 \end{pmatrix} \)

(7) \( \begin{pmatrix} m' \\ x,0,z \end{pmatrix} \)

(8) \( \begin{pmatrix} m' \\ 0,y,z \end{pmatrix} \)

For (1/2,1/2,1/2) + set

(1) \( \begin{pmatrix} t \end{pmatrix} \)

(2) \( \begin{pmatrix} 2 \end{pmatrix} \)

(3) \( \begin{pmatrix} 2 \end{pmatrix} \)

(4) \( \begin{pmatrix} 2 \end{pmatrix} \)

(5) \( \begin{pmatrix} \bar{1} \end{pmatrix} \)

(6) \( \begin{pmatrix} n' \end{pmatrix} \)

(7) \( \begin{pmatrix} n' \end{pmatrix} \)

(8) \( \begin{pmatrix} n' \end{pmatrix} \)
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x, y, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x, y, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x, y, z [u,v,w]</td>
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<td></td>
<td>(7) x, y, z [u,v,w]</td>
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<tr>
<td></td>
<td>(8) x, y, z [u,v,w]</td>
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<tr>
<td>8 n .m'</td>
<td>x,y,0 [u,v,w]</td>
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<td>x, y, 0 [u,v,0]</td>
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<td>x, 0, z [u,0,w]</td>
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<td></td>
<td>x, 0, z [u,0,w]</td>
</tr>
<tr>
<td>8 l .m'</td>
<td>0, y, z [0,v,w]</td>
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<tr>
<td></td>
<td>0, y, z [0,v,w]</td>
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<td></td>
<td>0, y, z [0,v,w]</td>
</tr>
<tr>
<td>8 k .m'</td>
<td>1/4, 1, 1/4 [0,0,0]</td>
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<tr>
<td></td>
<td>3/4, 3/4, 1/4 [0,0,0]</td>
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<td>3/4, 1/4, 3/4 [0,0,0]</td>
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<td></td>
<td>1/4, 3/4, 3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 j m'm'2</td>
<td>1/2, 0, z [0,0,w]</td>
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<tr>
<td></td>
<td>1/2, 0, z [0,0,w]</td>
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<td>4 i m'm'2</td>
<td>0, 0, z [0,0,w]</td>
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<td>0, 0, z [0,0,w]</td>
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<tr>
<td>4 h m'2m'</td>
<td>0, y, 1/2 [0, v,0]</td>
</tr>
<tr>
<td></td>
<td>0, y, 1/2 [0, v,0]</td>
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<td>4 g m'2m'</td>
<td>0, y, 0 [0, v,0]</td>
</tr>
<tr>
<td></td>
<td>0, y, 0 [0, v,0]</td>
</tr>
<tr>
<td>4 f 2m'm'</td>
<td>x, 1/2, 0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x, 1/2, 0 [u,0,0]</td>
</tr>
<tr>
<td>4 e 2m'm'</td>
<td>x, 0, 0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x, 0, 0 [u,0,0]</td>
</tr>
<tr>
<td>2 d m'm'm'</td>
<td>1/2, 0, 1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c m'm'm'</td>
<td>1/2, 1/2, 0 [0,0,0]</td>
</tr>
<tr>
<td>2 b m'm'm'</td>
<td>0, 1/2, 1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a m'm'm'</td>
<td>0, 0, 0 [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2m'm'</th>
<th>Along [1,0,0]</th>
<th>c2m'm'</th>
<th>Along [0,1,0]</th>
<th>c2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
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</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>

71.5.625 - 2 - 1243
**Symmetry Operations**

**For (0,0,0) + set**

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(1) (0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>2</td>
<td>(2) (0,0,z)</td>
<td>(2_z) (0,0,0)</td>
</tr>
<tr>
<td>3</td>
<td>(2) (0,y,0)</td>
<td>(2_y) (0,0,0)</td>
</tr>
<tr>
<td>4</td>
<td>(2) (x,0,0)</td>
<td>(2_x) (0,0,0)</td>
</tr>
<tr>
<td>5</td>
<td>(1) (0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>6</td>
<td>(m) (x,y,0)</td>
<td>(m_z) (0,0,0)</td>
</tr>
<tr>
<td>7</td>
<td>(m) (x,0,z)</td>
<td>(m_y) (0,0,0)</td>
</tr>
<tr>
<td>8</td>
<td>(m) (0,y,z)</td>
<td>(m_x) (0,0,0)</td>
</tr>
</tbody>
</table>

**For \((1/2,1/2,1/2)' + set\)**

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(t') (1/2,1/2,1/2)</td>
<td>(0,0,1/4)</td>
</tr>
<tr>
<td>2</td>
<td>(2') (0,0,1/2)</td>
<td>(1/4,1/4,1/4)</td>
</tr>
<tr>
<td>3</td>
<td>(2') (0,1/2,0)</td>
<td>(1/4,1/4,1/4)</td>
</tr>
<tr>
<td>4</td>
<td>(2') (1/2,0,0)</td>
<td>(1/4,1/4,1/4)</td>
</tr>
<tr>
<td>5</td>
<td>(1/2,1/2,1/2)</td>
<td>(0,0,1/4)</td>
</tr>
<tr>
<td>6</td>
<td>(n') (1/2,1/2,0)</td>
<td>(0,0,1/4)</td>
</tr>
<tr>
<td>7</td>
<td>(n') (1/2,0,1/2)</td>
<td>(0,0,1/4)</td>
</tr>
<tr>
<td>8</td>
<td>(n') (0,1/2,1/2)</td>
<td>(0,0,1/4)</td>
</tr>
</tbody>
</table>

**Asymmetric unit**

\[0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16 o 1</td>
<td>x,y,z [u,v,w]</td>
<td>(2) (\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>8 n m</td>
<td>x,y,0 [0,0,w]</td>
<td>(3) (x,y,\bar{z} [\bar{u},\bar{v},w])</td>
</tr>
<tr>
<td>8 m l</td>
<td>x,0,z [0,v,0]</td>
<td>(4) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td>8 k (\bar{1})</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>(5) (\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>4 j mm2</td>
<td>1/2,0,z [0,0,0]</td>
<td>(6) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td>4 i mm2</td>
<td>0,0,z [0,0,0]</td>
<td>(7) (x,\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>4 h m2m</td>
<td>0,y,1/2 [0,0,0]</td>
<td>(8) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td>4 g m2m</td>
<td>0,y,0 [0,0,0]</td>
<td>8 n m</td>
</tr>
<tr>
<td>4 f 2mm</td>
<td>x,1/2,0 [0,0,0]</td>
<td>(3) (x,y,\bar{z} [\bar{u},\bar{v},0])</td>
</tr>
<tr>
<td>4 e 2mm</td>
<td>x,0,0 [0,0,0]</td>
<td>(4) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td>2 d mmm</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>(5) (\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>2 c mmm</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>(6) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td>2 b mmm</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>(7) (x,\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>2 a mmm</td>
<td>0,0,0 [0,0,0]</td>
<td>(8) (x,y,z [u,v,w])</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = b)</td>
<td>(b^* = c)</td>
</tr>
</tbody>
</table>

Origin at x,0,0

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = c)</td>
<td>(b^* = a)</td>
</tr>
</tbody>
</table>

Origin at 0,y,0
Orthorhombic

Asymmetric unit:

\( 0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \)

Symmetry Operations

For \((0,0,0) + \) set:

1. \( (1) \uparrow (0,0,0) \)
2. \( (2) 0,0,z \)
3. \( (3) 0,y,0 \)
4. \( (4) x,0,0 \)

For \((1/2,1/2,1/2)'+ \) set:

1. \( (1) (1/2,1/2,1/2) \)
2. \( (2) (0,1/2,1/2) \)
3. \( (3) (0,1/2,0) \)
4. \( (4) (1/2,0,0) \)

Origin at center \((m'mm)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions  
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 n .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 m .m</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 l m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 k 1</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,3/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td>4 j m'2'</td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 i m'2'</td>
<td>0,0,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 h m'2'm</td>
<td>0,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 g m'2'm</td>
<td>0,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,0 [0,0,w]</td>
</tr>
<tr>
<td>4 f 2mm</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 e 2mm</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d m'mm</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c m'mm</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b m'mm</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a m'mm</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2mm1'  
  \( a' = a \)  \( b' = b \)  
  Origin at 0,0,z

- Along [1,0,0] c\(_p\)2mm  
  \( a' = b \)  \( b' = c \)  
  Origin at x,0,0

- Along [0,1,0] c2mm1'  
  \( a' = c \)  \( b' = a \)  
  Origin at 0,y,0
Origin at center (m’m’m)

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. 1  (1 0,0,0)
2. 2  0,0,z  (2 0,0,0)
3. 2’ 0,y,0  (2 0,0,0)’
4. 2’ x,0,0  (2 0,0,0)’
5. 1  (0,0,0)  (1 0,0,0)’
6. m  x,y,0  (m 0,0,0)  (m 0,0,0)’
7. m’ x,0,z  (m 0,0,0)’
8. m’ 0,y,z  (m 0,0,0)’

For (1/2,1/2,1/2)’ + set

1. t’ (1/2,1/2,1/2)  (1 1/2,1/2,1/2)’
2. 2’ (0,0,1/2)  1/4,1/4,z  (2 1/2,1/2,1/2)’
3. 2 (0,1/2,0)  1/4,y,1/4  (2 1/2,1/2,1/2)
4. 2 (1/2,0,0)  x,1/4,1/4  (2 1/2,1/2,1/2)
5. 1’ 1/4,1/4,1/4  (1 1/2,1/2,1/2)’
6. n’ (1/2,1/2,0)  x,y,1/4  (m 1/2,1/2,1/2)’
7. n (1/2,0,1/2)  x,1/4,z  (m 1/2,1/2,1/2)
8. n (0,1/2,1/2)  1/4,y,z  (m 1/2,1/2,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
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<th>Coordinates</th>
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<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) x̅,y̅,z [u̅,v̅,w̅]</td>
<td></td>
</tr>
<tr>
<td>(3) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
<td></td>
</tr>
<tr>
<td>(4) x̄,ȳ,z̄ [ū,v̄,w̄]</td>
<td></td>
</tr>
<tr>
<td>(5) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
<td></td>
</tr>
<tr>
<td>(6) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
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</tr>
<tr>
<td>(7) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
<td></td>
</tr>
<tr>
<td>(8) x̅,y̅,z̅ [u̅,v̅,w̅]</td>
<td></td>
</tr>
<tr>
<td>8 n .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>x̄,ȳ,0 [0,0,w]</td>
<td></td>
</tr>
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<td>x̅,y̅,0 [0,0,w]</td>
<td></td>
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<tr>
<td>x̅,y̅,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 m .m'</td>
<td>x̅,0,z [u̅,0,w]</td>
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<tr>
<td>x̅,0,z [u̅,0,w]</td>
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<tr>
<td>x̅,0,z [u̅,0,w]</td>
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<td>x̅,0,z [u̅,0,w]</td>
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<tr>
<td>8 l .m</td>
<td>0,y,z [0,v,w]</td>
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<td>0,y,z [0,v,w]</td>
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<td>0,y,z [0,v,w]</td>
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<td>0,y,z [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 k 1</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
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<tr>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td></td>
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<tr>
<td>3/4,1/4,3/4 [0,0,0]</td>
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<tr>
<td>1/4,3/4,3/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 j m'm'2</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>1/2,0,z [0,0,w]</td>
<td></td>
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<td>4 i m'm'2</td>
<td>0,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>4 h m'2m</td>
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</tr>
<tr>
<td>4 g m'2m</td>
<td>0,y,0 [0,0,w]</td>
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<tr>
<td>0,y,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 f 2'm'm</td>
<td>x,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>x̅,1/2,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 e 2'm'm</td>
<td>x,0,0 [0,0,w]</td>
</tr>
<tr>
<td>x̅,0,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 d m'm'm</td>
<td>1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c m'm'm</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 b m'm'm</td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a m'm'm</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c_p'2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c b* = b</td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>c_p'-2'mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c b* = a</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (m’m’m’)  

Asymmetric unit  
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2  

Symmetry Operations  

For (0,0,0) + set  

(1) 1  
(1) [0,0,0]  
(2) 2 0,0,z  
(2) [0,0,0]  
(3) 2 0,y,0  
(3) [0,0,0]  
(4) 2 x,0,0  
(4) [0,0,0]  
(5) 1/4,1/4,1/4  
(6) m’ x,y,0  
(6) [0,0,0]  
(7) m’ x,0,z  
(7) [0,0,0]  
(8) m’ 0,y,z  
(8) [0,0,0]  

(1) m’ (1/2,1/2,1/2)  
(1) [1/2,1/2,1/2]  
(2) 2’ (0,0,1/2) 1/4,1/4,z  
(2) [1/2,1/2,1/2]  
(3) 2’ (0,1/2,0) 1/4,y,1/4  
(3) [1/2,1/2,1/2]  
(4) 2’ (1/2,0,0) x,1/4,1/4  
(4) [1/2,1/2,1/2]  

(5) m’ (1/4,1/4,1/4)  
(5) [1/2,1/2,1/2]  
(6) n (1/2,1/2,0) x,y,1/4  
(6) [1/2,1/2,1/2]  
(7) n (1/2,0,1/2) x,1/4,z  
(7) [1/2,1/2,1/2]  
(8) n (0,1/2,1/2) 1/4,y,z  
(8) [1/2,1/2,1/2]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>16 o</td>
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<td>(1/2,1/2,1/2) +</td>
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<tr>
<td>8 n</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
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<tr>
<td>8 m</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
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<td>0,y,z [0,v,w]</td>
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<td>1/4,1/4,1/4 [u,v,w]</td>
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<tr>
<td>4 j</td>
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<td>1/2,0,z [0,0,0]</td>
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<tr>
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<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<tr>
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<td>0,y,1/2 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 g</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>4 f</td>
<td>x,1/2,0 [u,0,0]</td>
<td>x,1/2,0 [u,0,0]</td>
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<td>x,0,0 [u,0,0]</td>
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<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
<td>2 c</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
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<td>0,0,0 [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1]  c_p 2m'm'  
Along [1,0,0]  c_p 2m'm'  
Along [0,1,0]  c_p 2m'm'  

a* = a  b* = b  
a* = b  b* = c  
a* = c  b* = a  

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0  

71.9.629 - 2 - 1251
Orthorhombic

Ibam

\[ \text{72.1.630} \]

mmm

\[ \text{l2/b2/a2/m} \]

**Origin** at center \((2/m)\) at \(cc2/m\)

**Asymmetric unit**

\[
0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}
\]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1\)
   \[
   (1|0,0,0)
   \]
2. \(2\)
   \[
   (2|0,0,0; 2z|0,0,0)
   \]
3. \(3\)
   \[
   (3|0,0,1/2; 2z|0,0,1/2)
   \]
4. \(4\)
   \[
   (4|x,0,1/4; 2x|0,0,1/2)
   \]
5. \(5\)
   \[
   (5|0,0,0; m|0,0,0)
   \]
6. \(6\)
   \[
   (6|x,y,0; m|0,0,0)
   \]
7. \(7\)
   \[
   (7|0,0,1/2; c|0,0,1/2)
   \]
8. \(8\)
   \[
   (8|0,0,1/2; c|0,0,1/2)
   \]

For \((1/2,1/2,1/2)\) + set

1. \(1\)
   \[
   (1|1/2,1/2,1/2)
   \]
2. \(2\)
   \[
   (2|0,1/2,0; 1/2,1/2,1/2)
   \]
3. \(3\)
   \[
   (3|1/2,0,0; 1/2,1/2,0)
   \]
4. \(4\)
   \[
   (4|1/2,0,0; 1/2,1/2,0)
   \]
5. \(5\)
   \[
   (5|1/2,1/2,1/2)
   \]
6. \(6\)
   \[
   (6|x,y,1/4; m|1/2,1/2,1/2)
   \]
7. \(7\)
   \[
   (7|x,1/4,0; m|1/2,1/2,1/2)
   \]
8. \(8\)
   \[
   (8|1/4,y,z; m|1/2,1/2,0)
   \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tr>
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<td>(3) x, y, -z +1/2 [u,v,w]</td>
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<tr>
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<td>(4) x, y, -z +1/2 [u,v,w]</td>
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</tr>
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<td>(6) x, y, -z [u,v,w]</td>
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<td>(7) x, y, -z +1/2 [u,v,w]</td>
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<td>(8) x, y, -z +1/2 [u,v,w]</td>
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<td>8 j</td>
<td>x, y, 0 [0,0,w]</td>
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<td></td>
<td>x, y, 1/2 [0,0,w]</td>
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<td>x, y, 1/2 [0,0,w]</td>
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<td>8 h</td>
<td>0, 0, z [0,0,w]</td>
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<td>0, 0, z +1/2 [0,0,w]</td>
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<td>0, 0, z +1/2 [0,0,w]</td>
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<tr>
<td>8 g</td>
<td>0, y, 1/4 [0,v,0]</td>
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<td>0, y, 3/4 [0,v,0]</td>
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<tr>
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<td>4 d</td>
<td>1/2, 0, 0 [0,0,w]</td>
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<td>1/2, 0, 1/2 [0,0,w]</td>
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<td>0, 0, 1/2 [0,0,w]</td>
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<tr>
<td>4 c</td>
<td>0, 0, 0 [0,0,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>1/2, 0, 1/4 [0,0,0]</td>
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<td>0, 0, 1/4 [0,0,0]</td>
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<tr>
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<td>0, 0, 3/4 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] c2mm1'
- Along [1,0,0] p2_2_2'mm'
- Along [0,1,0] p2_2_2'mm'
- Origin at 0,0,z

a* = a  b* = b

Origin at x,0,0

a* = c/2  b* = a/2

Origin at x,0,0

Origin at 0,y,0

72.1.630 - 2 - 1253
**Origin** at center (2/m1') at cc2/m1'

**Asymmetric unit**

\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \quad (0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2,0,0,0) \\
(5) & \quad \overline{1} \quad 0,0,0 \\
& \quad (\overline{1},0,0,0) \\
(6) & \quad \bar{m} \quad x,y,0 \\
& \quad (m_x,0,0,0) \\
(7) & \quad \bar{c} \quad (0,0,1/2) \quad x,0,z \\
& \quad (m_y,0,0,1/2) \\
(8) & \quad \bar{c} \quad (0,0,1/2) \quad 0,y,z \\
& \quad (m_y,0,0,1/2) \\
\end{align*}
\]

For \((1/2,1/2,1/2) + \text{set}\)

\[
\begin{align*}
(1) & \quad t \quad (1/2,1/2,1/2) \\
& \quad (1/2,1/2,1/2) \\
(2) & \quad 2 \quad (0,0,1/2) \quad 1/4,1/4,z \\
& \quad (2,1/2,1/2,1/2) \\
(5) & \quad \overline{1} \quad 1/4,1/4,1/4 \\
& \quad (\overline{1},1/2,1/2,1/2) \\
(6) & \quad n \quad (1/2,1/2,0) \quad x,y,1/4 \\
& \quad (m_z,1/2,1/2,1/2) \\
(7) & \quad \bar{a} \quad (1/2,0,0) \quad x,1/4,z \\
& \quad (m_y,1/2,1/2,0) \\
(8) & \quad \bar{b} \quad (0,1/2,0) \quad 1/4,y,z \\
& \quad (m_z,1/2,1/2,0) \\
\end{align*}
\]

For \((0,0,0)' + \text{set}\)

\[
\begin{align*}
(1) & \quad 1' \quad (0,0,0)' \\
& \quad (1,0,0,0)' \\
(2) & \quad 2' \quad 0,0,z \\
& \quad (2,0,0,0)' \\
(5) & \quad \overline{1}' \quad 0,0,0 \\
& \quad (\overline{1},0,0,0)' \\
(6) & \quad m' \quad x,y,0 \\
& \quad (m_z,0,0,0)' \\
(7) & \quad \bar{c}' \quad (0,0,1/2) \quad x,0,z \\
& \quad (m_y,0,0,1/2)' \\
(8) & \quad \bar{c}' \quad (0,0,1/2) \quad 0,y,z \\
& \quad (m_y,0,0,1/2)' \\
\end{align*}
\]

For \((1/2,1/2,1/2)' + \text{set}\)

\[
\begin{align*}
(1) & \quad t' \quad (1/2,1/2,1/2)' \\
& \quad (1/2,1/2,1/2)' \\
(2) & \quad 2' \quad (0,0,1/2) \quad 1/4,1/4,z \\
& \quad (2,1/2,1/2,1/2)' \\
(5) & \quad \overline{1}' \quad 1/4,1/4,1/4 \\
& \quad (\overline{1},1/2,1/2,1/2)' \\
(6) & \quad n' \quad (1/2,1/2,0) \quad x,y,1/4 \\
& \quad (m_z,1/2,1/2,1/2)' \\
(7) & \quad \bar{a}' \quad (1/2,0,0) \quad x,1/4,z \\
& \quad (m_y,1/2,1/2,0)' \\
(8) & \quad \bar{b}' \quad (0,1/2,0) \quad 1/4,y,z \\
& \quad (m_z,1/2,1/2,0)' \\
\end{align*}
\]

\[72.2.631 - 1 - 1254\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

| Multiplicity, Wyckoff letter, Site Symmetry. | Coordinates | |
|---------------------------------------------|-------------|
| 16 k 11' (1) x,y,z [0,0,0]                  | (0,0,0) + (1/2,1/2,1/2) + |
| (5) x,y,z [0,0,0]                           | (0,0,0)' + (1/2,1/2,1/2)' + |
| 8 j .m1' x,y,0 [0,0,0]                      | x,y,z [0,0,0] |
| 8 i .21' 0,1/2,z [0,0,0]                    | x,y,z+1/2 [0,0,0] |
| 8 h .21' 0,0,z [0,0,0]                      | 0,0,z+1/2 [0,0,0] |
| 8 g .2.1' 0,y,1/4 [0,0,0]                   | 0,y,3/4 [0,0,0] |
| 8 f 2..1' x,0,1/4 [0,0,0]                   | x,0,3/4 [0,0,0] |
| 8 e 1' 1/4,1/4,1/4 [0,0,0]                 | 3/4,1/4,1/4 [0,0,0] |
| 4 d .2/m1' 1/2,0,0 [0,0,0]                  | 1/2,0,1/2 [0,0,0] |
| 4 c .2/m1' 0,0,0 [0,0,0]                    | 0,0,1/2 [0,0,0] |
| 4 b 2221' 1/2,0,1/4 [0,0,0]                | 1/2,0,3/4 [0,0,0] |
| 4 a 2221' 0,0,1/4 [0,0,0]                   | 0,0,3/4 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] c2mm1'  
**a**' = **a**  
**b**' = **b**

Along [1,0,0] p2mm1'  
**a**' = **b**/2  
**b**' = **c**/2

Along [0,1,0] p2mm1'  
**a**' = **c**/2  
**b**' = **a**/2

Origin at 0,0,z

Origin at x,0,0

Origin at 0,y,0
Ib'am
72.3.632

m'mm
I2/b'2'/a2'/m

Orthorhombic

Origin at center (2'/m) at c'c2'/m

Asymmetric unit
0 < x < 1/4; 0 < y < 1/2; 0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

1. I
   1 0 0
   (1 0 0,0)

2. 2' 0 0,0,0
   (2z 0,0,0')

3. 2' 0,y,1/4
   (2z 0,0,1/2')

4. 2 x,0,1/4
   (2z 0,0,1/2)

5. T 0,0,0
   (0 0,0,0)

6. m x,y,0
   (m_z 0,0,0)

7. c (0,0,1/2) x,0,z
   (m_y 0,0,1/2)

8. c' (0,0,1/2) 0,y,z
   (m_z 0,0,1/2')

For (1/2,1/2,1/2) + set

1. t (1/2,1/2,1/2)
   (1 1/2,1,1/2)

2. 2' (0,0,1/2) 1/4,1/4,z
   (2z 1/2,1/2,1/2')

3. 2' (0,1/2,0) 1/4,y,0
   (2z 1/2,1/2,0')

4. 2 (1/2,0,0) x,1/4,0
   (2z 1/2,1/2,0)

5. T 1/4,1/4,1/4
   (0 1/2,1/2,1/2)

6. n (1/2,1/2,0) x,y,1/4
   (m_z 1/2,1/2,1/2)

7. a (1/2,0,0) x,1/4,z
   (m_y 1/2,1/2,0)

8. b' (0,1/2,0) 1/4,y,z
   (m_z 1/2,1/2,0')
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<tr>
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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>16 k 1</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td>16 k 1</td>
<td>(3) x,y,z +1/2 [u,v,w]</td>
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<td>(4) x,y,z +1/2 [u,v,w]</td>
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<td>16 k 1</td>
<td>(5) x,y,z [u,v,w]</td>
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<td>x,y,0 [0,0,w]</td>
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<tr>
<td>8 i .2'</td>
<td>0,1/2,z [u,v,0]</td>
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<tr>
<td>8 h .2'</td>
<td>0,0,z [u,v,0]</td>
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</tr>
<tr>
<td>8 g .2'</td>
<td>0,y,1/4 [u,0,w]</td>
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<td>8 e .1'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
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<td>4 d .2'lm</td>
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<td>4 c .2'lm</td>
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<td>4 a 22'2'</td>
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Coordinates

(0,0,0) + (1/2,1/2,1/2) +

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<td>x</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1'  
Along [1,0,0] p2mm  
Along [0,1,0] p2mm  

a* = a  b* = b  
a* = b/2  b* = c/2  
a* = c/2  b* = a/2  

Origin at 0,0,z  
Origin at x,0,0
Ibam’  Orthorhombic

72.4.633  mmm’  l2'/b2'/a2/m’

Origin at center (2/m’) at cc2/m’

Asymmetric unit  0 ≤ x ≤ 1/4;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. \[ T (0,0,0) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

2. \[ T (0,0,z) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & z \end{bmatrix} \]

3. \[ T (0,y,1/4) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

4. \[ T (x,0,1/4) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

For (1/2,1/2,1/2) + set

1. \[ T (1/2,1/2,1/2) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

2. \[ T (0,0,1/2) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

3. \[ T (0,1/2,0) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]

4. \[ T (1/2,0,0) \]
   \[ \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z +1/2 [u,v,w]</td>
</tr>
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<td>(4) x,y,z +1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 j ..m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 i ..2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z +1/2 [0,0,w]</td>
</tr>
<tr>
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<td>0,1/2,z +1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 h ..2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z +1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z +1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 g ..2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [u,0,w]</td>
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<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>8 f ..2'</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
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<tr>
<td>8 e ..'</td>
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<tr>
<td></td>
<td>3/4,3/4,1/4 [0,0,0]</td>
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<tr>
<td></td>
<td>3/4,3/4,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] c2mm
- Along [1,0,0] p2m'm'
- Along [0,1,0] p2m'm'

```
<table>
<thead>
<tr>
<th>a' = a</th>
<th>b' = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = -c/2</td>
<td>b' = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>
```

```
<table>
<thead>
<tr>
<th>a' = a</th>
<th>b' = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = c/2</td>
<td>b' = a/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>
```

```
<table>
<thead>
<tr>
<th>a' = a</th>
<th>b' = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = c/2</td>
<td>b' = a/2</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
```
**Ib’a’m**

72.5.634

**m’m’m**

l2'/b'2'/a'2/m

**Orthorhombic**

**Origin** at center (2/m) at c’c’2/m

**Asymmetric unit**

\[0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

**Symmetry Operations**

**For (0,0,0) + set**

1. \(1\)
   
   \[x,0,0\]
   
   \[x,0,0\]
   
   \[x,0,0\]

2. \(2\)
   
   \[0,0,z\]
   
   \[0,0,z\]
   
   \[0,0,z\]

3. \(2’\)
   
   \[y,1/4\]
   
   \[y,1/4\]
   
   \[y,1/4\]

4. \(2’\)
   
   \[x,1/4\]
   
   \[x,1/4\]
   
   \[x,1/4\]

5. \(1\)
   
   \[m\]
   
   \[m\]
   
   \[m\]

6. \(6\)
   
   \[x,y,0\]
   
   \[x,y,0\]
   
   \[x,y,0\]

7. \(c’\)
   
   \[0,0,1/2\]
   
   \[0,0,1/2\]
   
   \[0,0,1/2\]

8. \(c’\)
   
   \[0,0,1/2\]
   
   \[0,0,1/2\]
   
   \[0,0,1/2\]

**For (1/2,1/2,1/2) + set**

1. \(1\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]

2. \(2\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]

3. \(2’\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]

4. \(2’\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]

5. \(1\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]

6. \(6\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]

7. \(a’\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]

8. \(b’\)
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
   
   \[1/2,1/2,1/2\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>(16) k (1)</td>
<td>((1)) (x,y,z) ([u,v,w])</td>
</tr>
<tr>
<td>(16) l (5)</td>
<td>((5)) (x,y,z) ([u,v,w])</td>
</tr>
<tr>
<td>(8) j (1)</td>
<td>((2)) (x,y,z) ([u,v,w])</td>
</tr>
<tr>
<td>(8) i (1)</td>
<td>((3)) (x,y,z+1/2) ([u,v,w])</td>
</tr>
<tr>
<td>(8) h (1)</td>
<td>((4)) (x,y,z+1/2) ([u,v,w])</td>
</tr>
<tr>
<td>(8) g (1)</td>
<td>((6)) (x,y,z) ([u,v,w])</td>
</tr>
<tr>
<td>(8) f (1)</td>
<td>((7)) (x,y,z+1/2) ([u,v,w])</td>
</tr>
<tr>
<td>(8) e (1)</td>
<td>((8)) (x,y,z+1/2) ([u,v,w])</td>
</tr>
<tr>
<td>(4) d (2/m)</td>
<td>((0,0,0))</td>
</tr>
<tr>
<td>(4) c (2/m)</td>
<td>((0,0,0))</td>
</tr>
<tr>
<td>(4) b (2'2')</td>
<td>((0,0,0))</td>
</tr>
<tr>
<td>(4) a (2'2')</td>
<td>((0,0,0))</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) c2mm1' Along \([1,0,0]\) p2'mm' Along \([0,1,0]\) p2'mm'  
\(a^* = a\) \(b^* = b\) \(a^* = c/2\) \(b^* = b/2\) \(a^* = c/2\) \(b^* = a/2\)  
Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Iba’m’ Orthorhombic
72.6.635

Origin at center (2’m’) at cc’2’m’

Asymmetric unit
0 < x < 1/4; 0 < y < 1/2; 0 < z < 1/2

Symmetry Operations

For (0,0,0) + set
(1) 1
(1 0,0,0)
(2) 2’ 0,0,z
(2z 0,0,0)’
(5) 1/4,0,0
(1/4 0,0,0)
(6) m’ x,y,0
(mz 0,0,0)’
(7) c’ (0,0,1/2) x,0,z
(my 0,0,1/2)’
(8) c (0,0,1/2) 0,y,z
(nz 0,0,1/2)

For (1/2,1/2,1/2) + set
(1) t (1/2,1/2,1/2)
(1/2 1/2,1/2,1/2)
(2) 2’ (0,0,1/2) 1/4,1/4,z
(2z 1/2,1/2,1/2)’
(6) n’ (1/2,1/2,0) x,y,1/4
(mz 1/2,1/2,1/2)’
(7) a’ (1/2,0,0) x,1/4,z
(my 1/2,1/2,0)’
(8) b (0,1/2,0) 1/4,y,z
(nz 1/2,1/2,0)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>8 j</td>
<td>x,y,0 [u,v,0]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 i</td>
<td>0,1/2,z [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 h</td>
<td>0,0,z [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 g</td>
<td>0,y,1/4 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 f</td>
<td>x,0,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 e</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 d</td>
<td>1/2,0,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 c</td>
<td>0,0,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>4 b</td>
<td>1/2,0,1/4 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,1/4 [u,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]   c2'mm'  Along [1,0,0]   p_{12}2mm  Along [0,1,0]   p2'mm'
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \quad \mathbf{a}^* = -\mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \quad \mathbf{a}^* = -\mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)

Origin at 0,0,z  Origin at x,0,1/4  Origin at 0,y,0
Ib'a'm' Orthorhombic
72.7.636

m'm'm' I2/b'2/a'2/m'

Origin at center (2/m') at c'c'/2/m'

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) \( \bar{1} \) 0,0,0
(1 | 0,0,0)
(2) \( 2 \) 0,0,z
(2_z | 0,0,0)
(3) \( 2 \) 0,y,1/4
(2_y | 0,0,1/2)
(4) \( 2 \) x,0,1/4
(2_x | 0,0,1/2)
(5) \( \bar{1} \) 0,0,0
(1 | 0,0,0)
(6) \( m' \) x,y,0
(m_z | 0,0,0)
(7) \( c' \) (0,0,1/2) x,0,z
(m_y | 0,0,1/2)
(8) \( c' \) (0,0,1/2) 0,y,z
(m_z | 0,0,1/2)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)
(2) \( 2 \) (0,0,1/2) 1/4,1/4,z
(2_z | 1/2,1/2,1/2)
(3) \( 2 \) (0,1/2,0) 1/4,y,0
(2_y | 1/2,1/2,0)
(4) \( 2 \) (1/2,0,0) x,1/4,0
(2_x | 1/2,1/2,0)
(5) \( \bar{1} \) 1/4,1/4,1/4
(1 | 1/2,1/2,1/2)
(6) n' (1/2,1/2,0) x,y,1/4
(m_z | 1/2,1/2,1/2)
(7) \( a' \) (1/2,0,0) x,1/4,z
(m_y | 1/2,1/2,0)
(8) \( b' \) (0,1/2,0) 1/4,y,z
(m_z | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 j</td>
<td>.m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>.2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>.2</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>.2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 f</td>
<td>2..</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>8 e</td>
<td>1/1</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>.2/m'</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>.2/m'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>222</td>
<td>1/2,0,1/4 [0,0,0]</td>
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<tr>
<td>4 a</td>
<td>222</td>
<td>0,0,1/4 [0,0,0]</td>
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### Coordinates

<table>
<thead>
<tr>
<th>(0,0,0) +</th>
<th>(1/2,1/2,1/2) +</th>
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<tbody>
<tr>
<td>16 k</td>
<td>8 j</td>
</tr>
<tr>
<td>8 i</td>
<td>8 h</td>
</tr>
<tr>
<td>8 g</td>
<td>8 f</td>
</tr>
<tr>
<td>8 e</td>
<td>4 d</td>
</tr>
<tr>
<td>4 c</td>
<td>4 b</td>
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<tr>
<td>4 a</td>
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</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2m'm'</th>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
<th>Along [0,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c/2</td>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at 0,y,0
IPbam

72.8.637

Orthorhombic

mmm1'

I2/b2/a2/m

Origin at center (2/m) at cc2/m

Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1

(1 | 0,0,0)

(2) 2 0,0,z

(2 | 0,0,0)

(3) 2 0,y,1/4

(2 | 0,0,1/2)

(4) 2 0,x,1/4

(2 | 0,0,1/2)

(5) m 0,0,0

(1 | 0,0,0)

(6) m x,y,0

(m_z | 0,0,0)

(7) c (0,0,1/2) x,0,z

(m_y | 0,0,1/2)

(8) c (0,0,1/2) 0,y,z

(m_z | 0,0,1/2)

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)

(1 | 1/2,1/2,1/2)

(2) 2' (0,0,1/2) 1/4,1/4,z

(2 | 1/2,1/2,1/2)

(3) 2' (0,1/2,0) 1/4,y,0

(2 | 1/2,1/2,0)

(4) 2' (1/2,0,0) x,1/4,0

(2 | 1/2,1/2,0)

(5) n' (1/2,1/2,0) x,y,1/4

(1 | 1/2,1/2,1/2)

(6) m' (1/2,1/2,0) x,y,1/4

(m_z | 1/2,1/2,1/2)

(7) a' (1/2,0,0) x,1/4,z

(m_y | 1/2,1/2,0)

(8) b' (0,1/2,0) 1/4,y,z

(m_z | 1/2,1/2,0)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)′ +</td>
<td></td>
</tr>
<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) x,y,z+1/2 [u,v,w]</td>
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<td>(4) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(7) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 j .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [0,0, w]</td>
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<tr>
<td>8 i .2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
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<td>0,1/2,z+1/2 [0,0, w]</td>
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<td>0,0,z+1/2 [0,0, w]</td>
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<tr>
<td>8 g .2</td>
<td>0,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,y,3/4 [0,v,0]</td>
</tr>
<tr>
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</tr>
<tr>
<td>8 f 2</td>
<td>x,0,1/4 [u,0,0]</td>
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<tr>
<td>8 e T′</td>
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<tr>
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<tr>
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</tr>
<tr>
<td>4 d .2/m</td>
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</tr>
<tr>
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<tr>
<td>4 b 222</td>
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<tr>
<td>4 a 222</td>
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</tr>
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<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c2mm1′
Along [1,0,0] p212′mm′
Along [0,1,0] p212′mm′

\[ a^* = a \quad b^* = b \]
\[ a^* = c/2 \quad b^* = b/2 \]
\[ a^* = c/2 \quad b^* = a/2 \]

Origin at 0,0,z
Origin at x,0,0
Origin at 0,y,0
Ip'b'am
Orthorhombic
72.9.638

$m\text{mm}1'$
$I_p2/b'2'/a2'/m$

Origin at center ($2'/m$) at $c'c'/m$

Asymmetric unit

\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}\]

Symmetry Operations

For $(0,0,0) +$ set

(1) $I$

(1) $0,0,0$

(2) $2', 0,0,z$

(2) $2', 0,0,0'$

(3) $2', 0,y,1/4$

(3) $2', 0,y,1/4'$

(4) $2, x,0,1/4$

(5) $I$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/4,1/4,1/4$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

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(1) $1/2,1/2,1/2'$

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(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

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(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

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(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$

(1) $1/2,1/2,1/2'$

(5) $T$

(1) $1/2,1/2,1/2$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>(0,0,0)</td>
<td>(1/2,1/2,1/2)</td>
</tr>
<tr>
<td>8 j</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 i</td>
<td>0,1/2,z [u,v,0]</td>
<td>0,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,0,z [u,v,0]</td>
<td>0,0,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>x,0,1/4 [u,0,0]</td>
<td>x,0,3/4 [u,0,0]</td>
</tr>
<tr>
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<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
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<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>4 b</td>
<td>1/2,0,1/4 [u,0,0]</td>
<td>1/2,0,3/4 [u,0,0]</td>
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<td>0,0,1/4 [u,0,0]</td>
<td>0,0,3/4 [u,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p_{2a}2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
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</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p_{2a}2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (2/m') at cc2/m'

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)
(2) 2 0,0,z (2z|0,0,0)
(3) 2' 0,y,1/4 (2y|0,0,1/2)
(4) 2' x,0,1/4 (2x|0,0,1/2)
(5) 1/4,1/4,0 (1/4,1/4,0)
(6) m' x,y,0 (mz|0,0,0)
(7) c (0,0,1/2) x,0,z (m,0,0,1/2)
(8) c (0,0,1/2) 0,y,z

For (1/2,1/2,1/2) + set

(1) t' (1/2,1/2,1/2) (1/2,1/2,1/2)
(2) 2' (0,0,1/2) 1/4,1/4,z (2z|1/2,1/2,1/2)
(3) 2 (0,1/2,0) 1/4,y,0 (2y|1/2,1/2,0)
(4) 2 (1/2,0,0) x,1/4,0 (2x|1/2,1/2,0)
(5) 1/4,1/4,1/4 (1/4,1/4,1/4)
(6) n (1/2,1/2,0) x,y,1/4 (mz|1/2,1/2,1/2)
(7) a' (1/2,0,0) x,1/4,z (my|1/2,1/2,0)
(8) b' (0,1/2,0) 1/4,y,z (mx|1/2,1/2,0)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
</tr>
<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z +1/2 [u,v,w]</td>
<td>(4) x,y,z +1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td>[u,v,w]</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>8 j -m'</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 i .2</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 h .2</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 g .2''</td>
<td>0,y,1/4 [u,0,w]</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 f .2''</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>8 e 1/4</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td>4 d .2/m'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2/m'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2'2'</td>
<td>1/2,0,1/4 [0,0,w]</td>
<td>1/2,0,3/4 [0,0,w]</td>
</tr>
<tr>
<td>4 a 2'2'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] c\_p\_2mm

\(a^* = a\) \(b^* = b\)

Origin at 0,0,z

Along [1,0,0] \(p_{2z2m'm'}\)

\(a^* = -c/2\) \(b^* = b/2\)

Origin at x,0,0

Along [0,1,0] \(p_{2z2m'm'}\)

\(a^* = c/2\) \(b^* = a/2\)

Origin at 0,y,0
Origin at center (2/m) at c'c'2/m

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For (0,0,0) + set

1) \[ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]

2) \[ \begin{pmatrix} 2 \\ 0,0,z \end{pmatrix} \]

3) \[ \begin{pmatrix} 2' \\ 0,y,1/4 \end{pmatrix} \]

4) \[ \begin{pmatrix} 2' \\ x,0,1/4 \end{pmatrix} \]

5) \[ \begin{pmatrix} 1/2,1/2,1/2 \end{pmatrix} \]

6) \[ \begin{pmatrix} m \\ x,y,0 \end{pmatrix} \]

7) \[ \begin{pmatrix} c' \end{pmatrix} \]

8) \[ \begin{pmatrix} c' \end{pmatrix} \]

For (1/2,1/2,1/2)' + set

1) \[ \begin{pmatrix} 1/2,1/2,1/2 \end{pmatrix} \]

2) \[ \begin{pmatrix} 2' \end{pmatrix} \]

3) \[ \begin{pmatrix} 2 \end{pmatrix} \]

4) \[ \begin{pmatrix} 2 \end{pmatrix} \]

5) \[ \begin{pmatrix} 1/4,1/4,1/4 \end{pmatrix} \]

6) \[ \begin{pmatrix} n' \end{pmatrix} \]

7) \[ \begin{pmatrix} a \end{pmatrix} \]

8) \[ \begin{pmatrix} b \end{pmatrix} \]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
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<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(2) x,y,z [u,v,w]</td>
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<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td>8 j .m</td>
<td>x,y,0 [0,0,w]</td>
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<td>x,y,0 [0,0,w]</td>
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<td>0,1/2,z +1/2 [0,0,w]</td>
</tr>
<tr>
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<td>0,1/2,z +1/2 [0,0,w]</td>
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<tr>
<td>8 h .2</td>
<td>0,0,z [0,0,w]</td>
</tr>
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<td>0,0,z [0,0,w]</td>
</tr>
<tr>
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<td>0,0,z +1/2 [0,0,w]</td>
</tr>
<tr>
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<td>0,0,z +1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 g .2'</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
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<td>0,y,3/4 [u,0,w]</td>
</tr>
<tr>
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<td>0,y,3/4 [u,0,w]</td>
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<tr>
<td>8 f .2'</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
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<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
</tr>
<tr>
<td>8 e .1'</td>
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<td>1/4,1/4,1/4 [0,0,0]</td>
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<tr>
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<td>3/4,3/4,1/4 [0,0,0]</td>
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<tr>
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<td>3/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 d .2/m</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
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<td></td>
<td>1/2,0,1/2 [0,0,w]</td>
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<tr>
<td>4 c .2/m</td>
<td>0,0,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 b 2'2'</td>
<td>1/2,0,1/4 [0,0,w]</td>
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<td>1/2,0,3/4 [0,0,w]</td>
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<tr>
<td>4 a 2'2'</td>
<td>0,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  c2mm1'  
Along [1,0,0]  p2121m'  
Along [0,1,0]  p2121m'  
Along [0,1,0]  p2121m'  
a* = a  b* = b  
a* = b/2  b* = c/2  
a* = -a/2  b* = c/2  
Origin at 0,0,z  
Origin at x,0,1/4  
Origin at 0,y,1/4
Origin at center ($2'm'$) at $c'c2'm'$

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2', 0,0,z \\
(3) & \quad 2 \quad 0,y,1/4 \\
(4) & \quad 2', x,0,1/4 \\
(5) & \quad m' \quad x,y,0 \\
(6) & \quad m \quad x,y,0 \\
(7) & \quad c \quad (0,0,1/2) \quad x,0,z \\
(8) & \quad c' \quad (0,0,1/2) \quad 0,y,z
\end{align*}
\]

For \((1/2,1/2,1/2)'\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad (0,0,1/2) \quad 1/4,1/4,1/4 \\
(3) & \quad 2' \quad (0,1/2,0) \quad 1/4,y,0 \\
(4) & \quad 2 \quad (1/2,0,0) \quad x,1/4,0 \\
(5) & \quad 1/2,1/2,1/2 \\
(6) & \quad n \quad (1/2,1/2,0) \quad x,y,1/4 \\
(7) & \quad a' \quad (1/2,0,0) \quad x,1/4,z \\
(8) & \quad b \quad (0,1/2,0) \quad 1/4,y,z
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
</tbody>
</table>

| 16 | k | 1 | (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] | (3) x,y,z +1/2 [u,v,w] | (4) x,y,z +1/2 [u,v,w] |
|    |   |   | (5) x,y,z [u,v,w] | (6) x,y,z [u,v,w] | (7) x,y,z +1/2 [u,v,w] | (8) x,y,z +1/2 [u,v,w] |
| 8  | j | ..m' | x,y,0 [u,v,0] | x,y,0 [u,v,0] | x,y,1/2 [u,v,0] | x,y,1/2 [u,v,0] |
| 8  | i | ..2' | 0,1/2,z [u,v,0] | 0,1/2,z [u,v,0] | 0,1/2,z +1/2 [u,v,0] | 0,1/2,z +1/2 [u,v,0] |
| 8  | h | ..2' | 0,0,z [u,v,0] | 0,0,z [u,v,0] | 0,0,z +1/2 [u,v,0] | 0,0,z +1/2 [u,v,0] |
| 8  | g | .2. | 0,y,1/4 [0,v,0] | 0,y,1/4 [0,v,0] | 0,y,3/4 [0,v,0] | 0,y,3/4 [0,v,0] |
| 8  | f | 2'. | x,0,1/4 [0,v,w] | x,0,1/4 [0,v,w] | x,0,3/4 [0,v,w] | x,0,3/4 [0,v,w] |
| 8  | e | 1/4,1,1/4 [0,0,0] | 1/4,3,4/4 [0,0,0] | 3/4,3,4/4 [0,0,0] | 3/4,1,4/4 [0,0,0] |
| 4  | d | ..2'm' | 1/2,0,0 [u,v,0] | 1/2,0,1/2 [u,v,0] |               |               |
| 4  | c | ..2'm' | 0,0,0 [u,v,0] | 0,0,1/2 [u,v,0] |               |               |
| 4  | b | 2'2' | 1/2,0,1/4 [0,v,0] | 1/2,0,3/4 [0,v,0] |               |               |
| 4  | a | 2'2' | 0,0,1/4 [0,v,0] | 0,0,3/4 [0,v,0] |               |               |

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>c_p 2'2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = -b</td>
<td>b^* = a</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p_2z 2'2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = b/2</td>
<td>b^* = c/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p_2z 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = c/2</td>
<td>b^* = a/2</td>
</tr>
<tr>
<td>Origin at 0,y,1/4</td>
<td></td>
</tr>
</tbody>
</table>
**Orthonhobic**

72.13.642

### Symmetry Operations

#### For (0,0,0) + set

1. $T(0,0,0)$
2. $2 \cdot 0,0,z$
3. $2 \cdot 0,y,1/4$
4. $2 \cdot x,0,1/4$
5. $m' \cdot 0,0,0$
6. $m' \cdot x,y,0$
7. $c' \cdot (0,0,1/2)$
8. $c' \cdot (0,0,1/2)$

#### For (1/2,1/2,1/2) + set

1. $t' (1/2,1/2,1/2)$
2. $2' (0,0,1/2) \cdot 1/4,1/4,z$
3. $2' (0,1/2,0) \cdot 1/4,y,0$
4. $2' (1/2,0,0) \cdot x,1/4,0$
5. $n (1/2,1/2,0) \cdot x,y,1/4$
6. $a (1/2,0,0) \cdot x,1/4,z$
7. $b (0,1/2,0) \cdot 1/4,y,z$
8. $m' (1/2,1/2,1/2)$

### Asymmetric unit

$$0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1/2$$
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 16 \ k \ 1 ) x,y,z [u,v,w] ( (1) )</td>
<td>( (0,0,0) + ) (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>( 8 \ j \ ..m' ) x,y,0 [u,v,0] ( (5) )</td>
<td>( \bar{x},y,\bar{z} [\bar{u},\bar{v},\bar{w}] )</td>
</tr>
<tr>
<td>( 8 \ i \ ..2 ) 0,1/2,z [0,0,w] ( (6) )</td>
<td>( \bar{x},y,\bar{z} [u,v,w] )</td>
</tr>
<tr>
<td>( 8 \ h \ ..2 ) 0,0,z [0,0,w] ( (7) )</td>
<td>( \bar{x},y,\bar{z}+1/2 [u,v,w] )</td>
</tr>
<tr>
<td>( 8 \ g \ ..2 ) 0,y,1/4 [0,v,0] ( (8) )</td>
<td>( \bar{x},y,\bar{z}+1/2 [\bar{u},\bar{v},\bar{w}] )</td>
</tr>
<tr>
<td>( 8 \ f \ .. ) ( x,0,1/4 [u,0,0] ) ( (1) )</td>
<td>( \bar{x},0,1/4 [\bar{u},0,0] )</td>
</tr>
<tr>
<td>( 8 \ e \ .. ) ( 1/4,1/4,1/4 [u,v,w] ) ( (1) )</td>
<td>( 1/4,3/4,1/4 [\bar{u},\bar{v},\bar{w}] )</td>
</tr>
<tr>
<td>( 4 \ d \ ..2/m' ) 1/2,0,0 [0,0,0] ( (1) )</td>
<td>( 1/2,0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>( 4 \ c \ ..2/m' ) 0,0,0 [0,0,0] ( (1) )</td>
<td>( 0,0,1/2 [0,0,0] )</td>
</tr>
<tr>
<td>( 4 \ b \ 222 ) 1/2,0,1/4 [0,0,0] ( (1) )</td>
<td>( 1/2,0,3/4 [0,0,0] )</td>
</tr>
<tr>
<td>( 4 \ a \ 222 ) 0,0,1/4 [0,0,0] ( (1) )</td>
<td>( 0,0,3/4 [0,0,0] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

\( \mathbf{a}^* = a \mathbf{b}^* = b \) Origin at 0,0,z

Along \( [0,0,1] \) c2m'm'

Along \( [1,0,0] \) \( p_{2a} \) 2m'm'

Along \( [0,1,0] \) \( p_{2a} \) 2m'm'

Along \( [0,1,0] \) \( p_{2a} \) 2m'm'

\( \mathbf{a}^* = -a/2 \mathbf{b}^* = c/2 \) Origin at x,0,0

\( \mathbf{a}^* = a/2 \mathbf{b}^* = c/2 \) Origin at 0,y,0
Ibca

73.1.643

Orthorhombic

mmm

I2_/b2_/c2_/a

Origin at \( \mathbf{1} \) at \( \mathbf{a} \mathbf{b} \mathbf{c} \)

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

Symmetry Operations

For \((0,0,0)\) + set

1. \( \mathbf{1} \)
2. \( (0,0,1/2) \quad 1/4,0,z \)
3. \( (0,1/2,0) \quad 0,y,1/4 \)
4. \( (1/2,0,0) \quad x,1/4,0 \)

5. \( \mathbf{1} \)
6. \( (0,0,0) \quad a \quad 1/2,0,1/2 \)
7. \( (0,1/2,0) \quad x,y,1/4 \)
8. \( (1/2,0,0) \quad m_z,1/2,0,1/2 \)

For \((1/2,1/2,1/2)\) + set

1. \( (1/2,1/2,1/2) \quad t \)
2. \( (1/2,1/2,0) \quad 0,1/4,z \)
3. \( (1/2,0,0) \quad 0,1/2,0 \)
4. \( (1/2,0,1/2) \quad 0,1/2,0 \)

5. \( \mathbf{1} \)
6. \( (0,1/2,0) \quad x,y,0 \)
7. \( (0,1/2,0) \quad x,0,z \)
8. \( (0,0,1/2) \quad z,0,1/4 \)

\( \mathbf{1} \mathbf{2} \mathbf{1} \mathbf{2} \mathbf{1} \mathbf{2} \)

\( m \mathbf{m} \mathbf{m} \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 f 1</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
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<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>8 e .2</td>
<td>0,1/4,z [0,0,w]</td>
</tr>
<tr>
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<td>0,3/4,z+1/2 [0,0,w]</td>
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<td>0,3/4,z [0,0,w]</td>
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<td>0,1/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 d .2</td>
<td>1/4,y,0 [0,v,0]</td>
</tr>
<tr>
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<td>1/4,y,1/2 [0,v,0]</td>
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<tr>
<td></td>
<td>3/4,y,0 [0,v,0]</td>
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<tr>
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<td>3/4,y,1/2 [0,v,0]</td>
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<tr>
<td>8 c 2..</td>
<td>x,0,1/4 [u,0,0]</td>
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<td>x+1/2,0,3/4 [u,0,0]</td>
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<tr>
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<td>x,0,3/4 [u,0,0]</td>
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<tr>
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<td>x+1/2,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>8 b 1</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
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<td>1/4,3/4,3/4 [u,v,w]</td>
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<td>3/4,1/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td>8 a 1</td>
<td>0,0,0 [u,v,w]</td>
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<td>1/2,0,1/2 [u,v,w]</td>
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<td>1/2,1/2,0 [u,v,w]</td>
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</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p c̄ 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a/2</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at 1/4,1/4,z</td>
<td>Origin at x,1/4,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p 2a̅ 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>p 2a̅ 2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c/2</td>
<td>b* = a/2</td>
</tr>
</tbody>
</table>

Continued
Ibca1' Orthorhombic

73.2.644 I2 1/b2 1/c2 1/a1'

Origin at 1 at abc

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 0 0 0)

(2) 2 (0,0,1/2) 1/4,0,z
(2z 1/2,0,1/2)

(3) 2 (0,1/2,0) 0,y,1/4
(2y 0,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2x 1/2,1/2,0)

(5) 1
(0 0,0 0)

(6) a (1/2,0,0) x,y,1/4
(mz 1/2,0,1/2)

(7) c (0,0,1/2) x,1/4,z
(my 0,1/2,1/2)

(8) b (0,1/2,0) 1/4,y,z
(mn 1/2,1/2,0)

For (1/2,1/2,1/2) + set

(1) 1
(1 1/2,1/2,1/2)

(2) 2 0,1/4,z
(2z 0,1/2,0)

(3) 2 1/4,y,0
(2y 0,1/2,0)

(4) 2 x,0,1/4
(2x 0,0,1/2)

(5) 1
(1/2,1/2,1/2)

(6) b (0,1/2,0) x,y,0
(mz 0,1/2,0)

(7) a (1/2,0,0) x,0,z
(my 1/2,0,0)

(8) c (0,0,1/2) 0,y,z
(mn 0,0,1/2)

For (0,0,0)' + set

(1) 1'
(1 0,0,0)'

(2) 2' (0,0,1/2) 1/4,0,z
(2z 1/2,0,1/2)'

(3) 2' (0,1/2,0) 0,y,1/4
(2y 0,1/2,1/2)'

(4) 2' (1/2,0,0) x,1/4,0
(2x 1/2,1/2,0)'

(5) 1'
(0 0,0 0)'

(6) a' (1/2,0,0) x,y,1/4
(mz 1/2,0,1/2)'

(7) c' (0,0,1/2) x,1/4,z
(my 0,1/2,1/2)'

(8) b' (0,1/2,0) 1/4,y,z
(mn 1/2,1/2,0)'

For (1/2,1/2,1/2)' + set

(1) 1'
(1 1/2,1/2,1/2)'

(2) 2' 0,1/4,z
(2z 0,1/2,0)'

(3) 2' 1/4,y,0
(2y 0,1/2,0)'

(4) 2' x,0,1/4
(2x 0,0,1/2)'

(5) 1'
(1/2,1/2,1/2)'

(6) b' (0,1/2,0) x,y,0
(mz 0,1/2,0)'

(7) a' (1/2,0,0) x,0,z
(my 0,1/2,0)'

(8) c' (0,0,1/2) 0,y,z
(mn 0,0,1/2)'
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + 11' x,y,z [0,0,0] &amp; (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
<tr>
<td>16 f 11' x+1/2,y,z [0,0,0] &amp; x+1/2,y+1/2,z+1/2 [0,0,0] &amp; x+1/2,y+1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 e 0.21' 0,1/4,z [0,0,0] &amp; 0,1/4,z+1/2 [0,0,0] &amp; 0,3/4,z [0,0,0] &amp; 0,1/4,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 d 0.21' 1/4,y,0 [0,0,0] &amp; 1/4,y+1/2 [0,0,0] &amp; 3/4,y,0 [0,0,0] &amp; 3/4,y,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 c 2.1' x,0,1/4 [0,0,0] &amp; x+1/2,0,3/4 [0,0,0] &amp; x,0,3/4 [0,0,0] &amp; x+1/2,0,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 b 21' 1/4,1/4,1/4 [0,0,0] &amp; 1/4,3/4,1/4 [0,0,0] &amp; 3/4,3/4,1/4 [0,0,0] &amp; 3/4,1/4,3/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 a 21' 0,0,0 [0,0,0] &amp; 1/2,0,1/2 [0,0,0] &amp; 0,1/2,1/2 [0,0,0] &amp; 1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p2mm1'  
  \(a^* = a/2\)  
  Origin at 0,0,z

- Along [1,0,0] p2mm1'  
  \(b^* = b/2\)  
  Origin at x,0,0

- Along [0,1,0] p2mm1'  
  \(c^* = c/2\)  
  Origin at 0,y,0
Ib'ca
73.3.645
Orthorhombic

m'mm
l2_and_b2_and_c2_and_a

Origin at c'ab

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. 1 (0,0,0)
   1 (0,0,0)

2. 2' (0,0,1/2) 1/4,0,z
   (2_z|1/2,0,1/2')

3. 2' (0,1/2,0) 0,y,1/4
   (2_y|0,1/2,1/2')

4. 2 (1/2,0,0) x,1/4,0
   (2_x|1/2,1/2,0)

5. 1' 0,0,0
   1 (0,0,0)

6. a (1/2,0,0) x,y,1/4
   (m_z|1/2,0,1/4)

7. c (0,0,1/2) x,1/4,z
   (m_y|1/2,1/4,1/4)

8. b' (0,1/2,0) 1/4,y,z
   (m_x|1/2,1/2,0)

For (1/2,1/2,1/2) + set

1. t (1/2,1/2,1/2)
   1 (1/2,1/2,1/2)

2. 2' 0,1/4,z
   (2_z|0,1/2,0)

3. 2' 1/4,y,0
   (2_y|1/2,0,0)

4. 2 x,0,1/4
   (2_x|0,0,1/2)

5. 1' 1/4,1/4,1/4
   1 (1/2,1/2,1/2)

6. b (0,1/2,0) x,y,0
   (m_z|0,1/2,0)

7. a (1/2,0,0) x,0,z
   (m_y|1/2,0,0)

8. c' (0,0,1/2) 0,y,z
   (m_x|0,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th></th>
<th>Coordinates</th>
<th></th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>16 f 1</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u,v,w]</td>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 e 2'</td>
<td>0,1/4,z [u,v,0]</td>
<td>8 d 2'</td>
<td>1/4,y,0 [u,0,w]</td>
</tr>
<tr>
<td>8 c 2'</td>
<td>x,0,1/4 [u,0,0]</td>
<td>8 d 2'</td>
<td>1/4,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 a 2'</td>
<td>0,0,0 [0,0,0]</td>
<td>8 d 2'</td>
<td>3/4,y,0 [u,0,w]</td>
</tr>
<tr>
<td>8 a 2'</td>
<td>0,0,0 [0,0,0]</td>
<td>8 d 2'</td>
<td>3/4,y,1/2 [u,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{2a}mm
\( a^* = a/2 \quad b^* = b/2 \)
Origin at 0,0,z

Along [1,0,0] p2mm
\( a^* = b/2 \quad b^* = c/2 \)
Origin at 0,0,0
**Ib'c'a m'm'm Orthorhombic**

73.4.646

<table>
<thead>
<tr>
<th>Origin</th>
<th>at 1 at c'a'b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asymmetric unit</td>
<td>0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

For (0,0,0) + set

1. $I (0,0,0)$
2. $2 (0,0,1/2) 1/4,0,z$
3. $2' (0,1/2,0) 0,y,1/4$
4. $2' (1/2,0,0) x,1/4,0$
5. $1/2,0,0)$
6. $a (1/2,0,0) x,y,1/4$
7. $c' (0,0,1/2) x,1/4,z$
8. $b' (0,1/2,0) 1/4,y,z$

For (1/2,1/2,1/2) + set

1. $t (1/2,1/2,1/2)$
2. $2 0,1/4,z$
3. $2' 1/4,y,0$
4. $2' x,0,1/4$
5. $1/2,1/2,1/2)$
6. $b (0,1/2,0) x,y,0$
7. $a' (1/2,0,0) x,0,z$
8. $c' (0,0,1/2) 0,y,z$

73.4.646 - 1 - 1284
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>8 e .2</td>
<td>0,1/4,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,3/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,3/4,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 d .2'</td>
<td>1/4,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 c 2'.</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,0,3/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>8 b 1</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/4,3/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td>8 a 1</td>
<td>0,0,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  \( p_{2a}.2m'm' \)

\[ a^* = a/2 \quad b^* = b/2 \]

Origin at 1/4,0,z

Along [1,0,0]  \( p2'mm' \)

\[ a^* = -c/2 \quad b^* = b/2 \]

Origin at x,0,0

Along [0,1,0]  \( p2'mm' \)

\[ a^* = c/2 \quad b^* = a/2 \]

Origin at 0,y,0
Ib'c'a'  
73.5.647

Orthorhombic

m'm'm'
I21/b21/c21/a'

Origin at 1 at cab
Asymmetric unit 
0 < x < 1/4;  0 < y < 1/2;  0 < z < 1/2

Symmetry Operations

For (0,0,0) + set

1 1
(1) 0,0,0
(2) 0,0,1/2 1/4,0,z
(3) 0,1/2,0 0,y,1/4
(4) 1/2,0,0 x,1/4,0

(5) T' 0,0,0
(1) 0,0,0
(2) (1/2,0,0) x,y,1/4
(3) (0,0,1/2) x,1/4,z
(4) (0,1/2,0) 1/4,y,z

5 (1) 1/2,1/2,1/2
(2) 0,1/4,z
(3) 1/4,y,0
(4) x,0,1/4

5 (1) 1/2,1/2,1/2
(2) 1/2,0,1/2
(3) 1/4,0,0
(4) 2,0,1/2

(5) T' 1/4,1/4,1/4
(1) 1/2,1/2,1/2
(2) 0,1/2,0 x,y,0
(3) 1/2,0,0 x,0,z
(4) 0,1/2,0 0,y,z
(5) 1/2,1/2,1/2
(6) 1/2,0,1/2
(7) 0,1/2,0
(8) 0,0,1/2
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td>16 f 1</td>
<td>( x,y,z \ [u,v,w] )</td>
<td>( u,v,w )</td>
</tr>
<tr>
<td>8 e .2</td>
<td>( 0,1/4,z \ [0,0,w] )</td>
<td>( 0,1/4,z+1/2 \ [0,0,w] )</td>
</tr>
<tr>
<td>8 d .2</td>
<td>( 1/4,y,0 \ [0,v,0] )</td>
<td>( 3/4,y,1/2 \ [0,v,0] )</td>
</tr>
<tr>
<td>8 c .2</td>
<td>( x,0,1/4 \ [u,0,0] )</td>
<td>( x+1/2,0,1/4 \ [u,0,0] )</td>
</tr>
<tr>
<td>8 b ( \bar{T'} )</td>
<td>( 1/4,1/4,1/4 \ [0,0,0] )</td>
<td>( 3/4,1/4,3/4 \ [0,0,0] )</td>
</tr>
<tr>
<td>8 a ( \bar{T'} )</td>
<td>( 0,0,0 \ [0,0,0] )</td>
<td>( 1/2,1/2,0 \ [0,0,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) p2m'\'m'
  - \( a' = a/2 \)
  - \( b' = b/2 \)
- Origin at \( 0,0,z \)
- Along \([1,0,0]\) p2m'\'m'
  - \( a' = b/2 \)
  - \( b' = c/2 \)
- Origin at \( x,0,0 \)
- Along \([0,1,0]\) p2m'\'m'
  - \( a' = c/2 \)
  - \( b' = a/2 \)
- Origin at \( 0,y,0 \)
Origin at \( \bar{1} \) at c'ab'

Asymmetric unit: 

\[
0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1/2
\]

Symmetry Operations

For \((0,0,0)\) + set

1. \( \bar{1} (0,0,0) \)
2. \( \bar{2} (0,0,1/2) 1/4,0,z \)
3. \( \bar{2} (0,1/2,0) 0,y,1/4 \)
4. \( \bar{2} (1/2,0,0) x,1/4,0 \)
5. \( 0,0,0 \)
6. \( a (1/2,0,0) x,y,1/4 \)
7. \( c (0,0,1/2) x,1/4,z \)
8. \( b (0,1/2,0) 1/4,y,z \)

For \((1/2,1/2,1/2)\)' + set

1. \( \bar{1} (1/2,1/2,1/2) \)
2. \( \bar{2} (0,0,1/2) 1/4,0,z \)
3. \( \bar{2} (0,1/2,0) 0,y,1/4 \)
4. \( \bar{2} (1/2,0,0) x,1/4,0 \)
5. \( 0,0,0 \)
6. \( a' (1/2,0,0) x,0,z \)
7. \( c' (0,0,1/2) 0,y,z \)
8. \( b' (0,1/2,0) x,y,0 \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Positions</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x+1/2,y,z+1/2 [u,v,w]</td>
<td>(7) x,y+1/2,z+1/2 [u,v,w]</td>
<td>(8) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 8 e .2'      | 0,1/4,0 [u,v,0] | 0,3/4,0 [u,v,0] | 0,3/4,0 [u,v,0] | 0,1/4,0 [u,v,0] |
| 8 d .2'      | 1/4,0,0 [u,v,w] | 1/4,0,0 [u,v,w] | 3/4,0,0 [u,v,w] | 3/4,0,0 [u,v,w] |
| 8 c 2'       | x,0,1/4 [0,v,w] | x+1/2,0,3/4 [0,v,w] | x,0,3/4 [0,v,w] | x+1/2,0,1/4 [0,v,w] |
| 8 b 1/4      | 1/4,1/4,1/4 [0,v,w] | 1/4,3/4,3/4 [0,v,w] | 3/4,3/4,3/4 [0,v,w] | 3/4,1/4,3/4 [0,v,w] |
| 8 a 1/4      | 0,0,0 [u,v,w] | 1/2,0,1/2 [u,v,w] | 0,1/2,1/2 [u,v,w] | 1/2,1/2,0 [u,v,w] |

## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p_{2a}2mm</th>
<th>Along [1,0,0] p_{2a}2mm</th>
<th>Along [0,1,0] p_{2a}2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a/2</td>
<td>b' = b/2</td>
<td>a' = c/2</td>
</tr>
<tr>
<td>Origin at 1/4,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at 0,y,1/4</td>
</tr>
</tbody>
</table>

73.6.648 - 2 - 1289
Orthorhombic

73.7.649

I\textsubscript{b}b'ca

mmm1'

I\textsubscript{2}2'/b'2'/c2'/a

Asymmetric unit

0\leq x \leq 1/4; 0\leq y \leq 1/2; 0\leq z \leq 1/2

Symmetry Operations

For (0,0,0) + set

(1) \text{1} \quad (1 \mid 0,0,0)

(2) \text{2}' \ (0,0,1/2) \ (1/4,0,z)

(3) \text{2}' \ (0,1/2,0) \ (0,y,1/4)

(4) \text{2} \ (1/2,0,0) \ (x,1/4,0)

(5) \text{1}' \ (0,0,0)

(1 \mid 0,0,0)'

(6) \ a \ (1/2,0,0) \ (x,y,1/4)

(7) \ c \ (0,0,1/2) \ (x,1/4,z)

(8) \ b' \ (0,1/2,0) \ (1/4,y,z)

For (1/2,1/2,1/2)' + set

(1) \text{t}' \ (1/2,1/2,1/2)

(1 \mid 1/2,1/2,1/2)'

(2) \ b' \ (0,1/2,0) \ (0,1/4,z)

(3) \ b' \ (0,1/2,0) \ (1/2,y,1/2,0)

(4) \text{2}' \ x,0,1/4

(2 \mid 0,0,1/2)'

(5) \text{1}' \ (1/4,1/4,1/4)

(1 \mid 2,1/2,1/2)'

(6) \ a' \ (1/2,0,0) \ x,y,0

(7) \ a' \ (1/2,0,0) \ x,0,z

(8) \ c \ (0,0,1/2) \ 0,y,z

(3 \mid 1/2,0,0)'

(4 \mid 0,0,1/2)'

73.7.649 - 1 - 1290
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Positions</th>
<th>Coordinates</th>
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<td>16 f 1</td>
<td>((0,0,0) + (1/2,1/2,1/2)' + (1/2,1/2,1/2))</td>
<td>((1)) x,y,z [u,v,w]</td>
<td>((2)) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 e ..2</td>
<td>0,1/4,z [0,0,w]</td>
<td>0,3/4,z+1/2 [0,0,w]</td>
<td>0,1/4,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 d .2</td>
<td>1/4,y,0 [0,v,0]</td>
<td>1/4,y,1/2 [0,v,0]</td>
<td>3/4,y,0 [0,v,0]</td>
</tr>
<tr>
<td>8 c 2'..</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x+1/2,0,3/4 [0,v,w]</td>
<td>x+1/2,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td>8 b 1</td>
<td>1/4,1,4,1/4 [u,v,w]</td>
<td>1/4,3/4,3/4 [u,v,w]</td>
<td>3/4,1/4,3/4 [u,v,w]</td>
</tr>
<tr>
<td>8 a 1'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \(p_{2a}2mm\) \(p_{2a}2m'm'\) \(p_{2a}2m'm'\)
\[a^* = a/2 \quad b^* = b/2\]
\[a^* = -c/2 \quad b^* = b/2\]
\[a^* = c/2 \quad b^* = a/2\]

Origin at 0,0,z Origin at x,0,0 Origin at 0,y,0
Imma
74.1.650

Orthorhombic

mmm
I2/m2/m2/a

Origin at center (2/m) at 2/m2/nb

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 0,1/4,z
(2 | 0,1/2,0)

(3) 2 (0,1/2,0) 0,y,0
(2 | 0,1/2,0)

(4) 2 x,0,0
(2 | 0,0,0)

(5) 1
(1 | 0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,0,z
(2 | 1/2,0,1/2)

(3) 2 1/4,y,1/4
(2 | 1/2,0,1/2)

(4) 2 (1/2,0,0) x,1/4,1/4
(2 | 1/2,1/2,1/2)

(5) 1
(1 | 0,0,0)

(6) a (1/2,0,0) x,y,1/4
(1 | 2,0,1/2)

(7) n (1/2,0,1/2) x,0,z
(1 | 2,0,1/2)

(8) n (0,1/2,1/2) 1/4,y,z
(1 | 2,1/2,1/2)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<table>
<thead>
<tr>
<th>16 j 1</th>
<th>(1) x,y,z [u,v,w] (2) x,y+1/2,z [u,v,w] (3) x,y+1/2,z [u,v,w] (4) x,y,z [u,v,w]</th>
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<tr>
<td>8 i .m.</td>
<td>8 x,1/4,z [0,v,0] x,1/4,z [0,v,0] x,3/4,z [0,v,0] x,3/4,z [0,v,0]</td>
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<td>8 h m..</td>
<td>8 0,y,z [u,0,0] 0,y+1/2,z [u,0,0] 0,y+1/2,z [u,0,0] 0,y,z [u,0,0]</td>
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<tr>
<td>8 g .2.</td>
<td>8 1/4,y,1/4 [0,v,0] 3/4,y+1/2,1/4 [0,v,0] 3/4,y+1/2,1/4 [0,v,0] 1/4,y+1/2,3/4 [0,v,0]</td>
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<tr>
<td>8 f .2..</td>
<td>8 x,0,0 [u,0,0] x,1/2,0 [u,0,0] x,0,0 [u,0,0] x,1/2,0 [u,0,0]</td>
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<tr>
<td>4 e mm2</td>
<td>4 0,1/4,z [0,0,0] 0,3/4,z [0,0,0]</td>
</tr>
<tr>
<td>4 d .2/m.</td>
<td>4 1/4,1/4,3/4 [0,v,0] 3/4,1/4,3/4 [0,v,0]</td>
</tr>
<tr>
<td>4 c .2/m.</td>
<td>4 1/4,1/4,3/4 [0,v,0] 3/4,1/4,3/4 [0,v,0]</td>
</tr>
<tr>
<td>4 b 2/m..</td>
<td>4 0,1/2 [u,0,0] 0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 a 2/m..</td>
<td>4 0,0,0 [u,0,0] 0,1/2,0 [u,0,0]</td>
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**Symmetry of Special Projections**

- Along [0,0,1] p2a 2mm  
  \( a^* = a/2 \quad b^* = b/2 \)
  Origin at 0,1/4,z

- Along [1,0,0] c2mm1'  
  \( a^* = b \quad b^* = c \quad a^* = c \quad b^* = a \)
  Origin at 0,y,0
Imma1'  
74.2.651  

**Orthorhombic**  

**mmm1'**  
l2_/m2_/m2_/a1'  

Origin at center (2/m1') at 2/m2_/nb1'

Asymmetric unit  
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

**Symmetry Operations**  

For (0,0,0) + set

1. **1** (0,0,0)  
2. **2** 0,1/4,z  
3. **2** (0,1/2,0) 0,y,0  
4. **2** x,0,0  

For (1/2,1/2,1/2) + set

5. **1/2,1/2,1/2**  
6. **2** (0,0,1/2) 1/4,0,z  
7. **2** 1/4,y,1/4  
8. **2** (1/2,0,0) 1/4,1/4,1/4

For (0,0,0)' + set

1'. **1/2,1/2,1/2**  
2'. **2**' 0,1/4,z  
3'. **2**' (0,1/2,0) 0,y,0  
4'. **2**' x,0,0  

For (1/2,1/2,1/2)' + set

5'. **1/2,1/2,1/2**  
6'. **2**' (0,1/2,0) 1/4,0,z  
7'. **2**' 1/4,y,1/4  
8'. **2**' (1/2,0,0) 1/4,1/4,1/4
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>16 j 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y+1/2,z [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>(3) x,y+1/2,z [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x,y,z [0,0,0]</td>
</tr>
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</table>

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<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>(0,0,0)' +</td>
<td>(1/2,1/2,1/2)' +</td>
</tr>
</tbody>
</table>

| 8 i .m.1'  | x,1/4,z [0,0,0] |
| 8 h .m..1' | 0,y,z [0,0,0] |
| 8 g .2.1'  | 1/4,y,1/4 [0,0,0] |
| 8 f .2..1' | x,0,0 [0,0,0] |
| 4 e mm1'   | 0,1/4,z [0,0,0] |
| 4 d .2/m.1' | 1/4,1/4,3/4 [0,0,0] |
| 4 c .2/m.1' | 1/4,1/4,1/4 [0,0,0] |
| 4 b 2/m..1' | 0,0,1/2 [0,0,0] |
| 4 a 2/m..1' | 0,0,0 [0,0,0] |

### Symmetry of Special Projections

- Along [0,0,1] p2mm1':
  - \( \mathbf{a}^* = \mathbf{a}/2 \)
  - \( \mathbf{b}^* = \mathbf{b}/2 \)
- Along [1,0,0] c2mm1':
  - \( \mathbf{a}^* = \mathbf{b} \)
  - \( \mathbf{b}^* = \mathbf{c} \)
- Along [0,1,0] c2mm1':
  - \( \mathbf{a}^* = \mathbf{c} \)
  - \( \mathbf{b}^* = \mathbf{a} \)
- Origin at 0,0,z
- Origin at x,1/4,1/4
- Origin at 0,y,0
Im' ma  
74.3.652  
m' mm  
l2, m'2, '/m2, '/a  
Orthorhombic

Origin at center (2/m') at 2/m'2, '/nb

Asymmetric unit  
0 < x < 1/4; 0 < y < 1/4; 0 < z < 1

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1 | 0,0,0)

(2) 2' 0,1/4,z  
(2z | 0,1/2,0)'

(3) 2' (0,1/2,0) 0,y,0  
(2 | 0,1/2,0)'

(4) 2 x,0,0  
(2x | 0,0,0)

(5) m' 0,0,0  
(m | 0,0,0)'

(6) b (0,1/2,0) x,y,0  
(mz | 0,1/2,0)

(7) m x,1/4,z  
(my | 0,1/2,0)

(8) m' 0,y,z  
(my | 0,0,0)'

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  
(1 | 1/2,1/2,1/2)

(2) 2' (0,0,1/2) 1/4,0,z  
(2z | 1/2,0,1/2)'

(3) 2' 1/4,y,1/4  
(2y | 1/2,0,1/2)'

(4) 2 (1/2,0,0) x,1/4,1/4  
(2x | 1/2,1/2,1/2)

(5) m' 1/4,1/4,1/4  
(mz | 1/2,0,1/2)'

(6) a (1/2,0,0) x,y,1/4  
(mz | 1/2,0,1/2)

(7) n (1/2,0,1/2) x,0,z  
(my | 1/2,0,1/2)

(8) n' (0,1/2,1/2) 1/4,y,z  
(my | 1/2,1/2,1/2)'
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 j</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y + 1/2, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u,v,w]</td>
<td>(6) x, y + 1/2, z [u,v,w]</td>
</tr>
<tr>
<td>8 i.m.</td>
<td>x, 1/4, z [0,v,0]</td>
<td>x, 3/4, z [0,v,0]</td>
</tr>
<tr>
<td>8 h m'..</td>
<td>0, y, z [0,v,w]</td>
<td>0, y + 1/2, z [0,v,w]</td>
</tr>
<tr>
<td>8 g .2'..</td>
<td>1/4, y, 1/4 [u,0,w]</td>
<td>3/4, y + 1/2, 1/4 [u,0,w]</td>
</tr>
<tr>
<td>8 f .2..</td>
<td>x, 0, 0 [u,0,0]</td>
<td>x, 1/2, 0 [u,0,0]</td>
</tr>
<tr>
<td>4 e m’m2'</td>
<td>0, 1/4, z [0,v,0]</td>
<td>0, 3/4, z [0,v,0]</td>
</tr>
<tr>
<td>4 d .2'/m.</td>
<td>1/4, 1/4, 3/4 [0,0,0]</td>
<td>3/4, 1/4, 3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2'/m.</td>
<td>1/4, 1/4, 1/4 [0,0,0]</td>
<td>3/4, 1/4, 1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2/m'..</td>
<td>0, 0, 1/2 [0,0,0]</td>
<td>0, 1/2, 1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2/m'..</td>
<td>0, 0, 0 [0,0,0]</td>
<td>0, 1/2, 0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1]  p_{2a}, 2m’m’  
  \( a^* = -b/2 \quad b^* = a/2 \)
- Along [1,0,0]  c2mm  
  \( a^* = b \quad b^* = c \)
- Along [0,1,0]  c2mm1’  
  \( a^* = c \quad b^* = a \)

Origin at 0,0,z  
Origin at x,1/4,1/4  
Origin at 0,y,0
Imma' 74.4.653

mmm' I2,'m2,'m2,'a'

Orthorhombic

Origin at center (2'/m) at 2'/m2,'nb'

Asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1 | 0,0,0)

(2) 2 0,1/4,z
    (2 | 0,1/2,0)

(3) 2' (0,1/2,0) 0,y,0
    (2' | 0,1/2,0)'

(4) 2' x,0,0
    (2' | 0,0,0)'

(5) 2 0,0,0
    (2 | 0,0,0)' (1 | 0,0,0)'

(6) b' (0,1/2,0) x,y,0
    (m | 0,1/2,0)'

(7) m x,1/4,z
    (m | 0,1/2,0)

(8) m 0,y,z
    (m | 0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
    (1 | 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,0,z
    (2 | 1/2,0,1/2)

(3) 2' 1/4,y,1/4
    (2' | 1/2,0,1/2)'

(4) 2' (1/2,0,0) x,1/4,1/4
    (2' | 1/2,1/2,1/2)'

(5) 2' 1/4,1/4,1/4
    (1 | 1/2,1/2,1/2)'

(6) a' (1/2,0,0) x,y,1/4
    (m | 1/2,0,1/2)'

(7) n (1/2,0,1/2) x,0,z
    (m | 1/2,0,1/2)

(8) n (0,1/2,1/2) 1/4,y,z
    (m | 1/2,1/2,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<tbody>
<tr>
<td>16 j</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 i m.</td>
<td>x,1/4,z [0,v,0]</td>
<td>[u,v,0]</td>
</tr>
<tr>
<td>8 h m..</td>
<td>0,y,z [u,0,0]</td>
<td>[u,0,0]</td>
</tr>
<tr>
<td>8 g .2'.</td>
<td>1/4,y,1/4 [u,0,w]</td>
<td>[u,0,w]</td>
</tr>
<tr>
<td>8 f .2'..</td>
<td>x,0,0 [0,v,w]</td>
<td>[u,0,w]</td>
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<tr>
<td>4 e mm2</td>
<td>0,1/4,z [0,0,0]</td>
<td>[0,0,0]</td>
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<tr>
<td>4 d .2'/m.</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>[0,0,0]</td>
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<tr>
<td>4 c .2'/m.</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>4 b 2'/m..</td>
<td>0,0,1/2 [0,0,0]</td>
<td>[0,0,0]</td>
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<tr>
<td>4 a 2'/m..</td>
<td>0,0,0 [0,0,0]</td>
<td>[0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]    p2mm        Along [1,0,0] c2mm1'       Along [0,1,0] c2mm1'
   \[a^* = a/2\] \[b^* = b/2\] \[a^* = b\] \[b^* = c\] \[a^* = c\] \[b^* = a\]
Origin at 0,0,z  Origin at x,1/4,1/4                  Origin at 0,y,0
Im'm'a

74.5.654

m'm'm

l2,/m'2,/m'2,/a

Orthorhombic

Origin at center (2'/m') at 2'/m'2,/m'b

Asymmetric unit

\[0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1\]

Symmetry Operations

For \((0,0,0) + \text{ set}\)

1. \(1\)
2. \(2 \quad 0,1/4,z\)
3. \(2' \quad (0,1/2,0)\)
4. \(2' \quad x,0,0\)
5. \(1\)
6. \(b \quad (0,1/2,0)\)
7. \(m' \quad x,1/4,z\)
8. \(m' \quad 0,y,z\)

For \((1/2,1/2,1/2) + \text{ set}\)

1. \(t \quad (1/2,1/2,1/2)\)
2. \(2 \quad (0,0,1/2)\)
3. \(2' \quad 1/4,y,1/4\)
4. \(2' \quad (1/2,0,0)\)
5. \(1\)
6. \(a \quad (1/2,0,0)\)
7. \(n' \quad (1/2,0,1/2)\)
8. \(n' \quad (0,1/2,1/2)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>(1/4,z) [u,0,w]</td>
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<td>8 h</td>
<td>(0,y,z) [0,v,w]</td>
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<td>8 g</td>
<td>(1/4,1/4) [u,0,w]</td>
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<td>4 e</td>
<td>(0,1/4,z) [0,0,w]</td>
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<tr>
<td>4 d</td>
<td>(1/4,1/4,3/4) [u,0,w]</td>
</tr>
<tr>
<td>4 c</td>
<td>(1/4,1/4,1/4) [u,0,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>(0,0,1/2) [0,v,w]</td>
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<tr>
<td>4 a</td>
<td>(0,0,0) [0,v,w]</td>
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Symmetry of Special Projections

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<tr>
<th>Along [0,0,1]</th>
<th>(p_{2a})2m'm'</th>
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<tbody>
<tr>
<td>(a^* = a/2)</td>
<td>(b^* = b/2)</td>
</tr>
<tr>
<td>Origin at 0,1/4,z</td>
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<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c2'2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = -c)</td>
<td>(b^* = b)</td>
</tr>
<tr>
<td>Origin at x,1/4,1/4</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [0,1,0]</th>
<th>c2'2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = c)</td>
<td>(b^* = a)</td>
</tr>
<tr>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Imm'a' mm'm' Orthorhombic

74.6.655 l2/m21'/m'/a'

Origin at center (2/m) at 2/m21'/n'b'

Asymmetric unit

0 < x < 1/4; 0 < y < 1/4; 0 < z < 1

Symmetry Operations

For (0,0,0) + set

(1) 1 (1 | 0,0,0)
(2) 2' 0,1/4,z (2 | 0,1/2,0')
(3) 2' (0,1/2,0) 0,y,0 (2 | 0,1/2,0')
(4) 2 x,0,0 (2 | 0,0,0)
(5) 1/2,1/2,1/2 (1 | 0,0,0)
(6) b' (0,1/2,0) x,y,0 (m_z | 1/2,0,1/2')
(7) m' x,1/4,z (m_y | 0,1/2,0')
(8) m 0,y,z (m_z | 0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1 | 1/2,1/2,1/2)
(2) 2' (0,0,1/2) 1/4,0,z (2 | 1/2,0,1/2')
(3) 2' 1/4,y,1/4 (2 | 1/2,0,1/2')
(4) 2 (1/2,0,0) x,1/4,1/4 (2 | 1/2,1/2,1/2)
(5) 1/4,1/4,1/4 (1 | 1/2,1/2,1/2)
(6) a' (1/2,0,0) x,y,1/4 (m_z | 1/2,0,1/2')
(7) n' (1/2,0,1/2) x,0,z (m_y | 1/2,0,1/2')
(8) n 0,1/2,1/2 1/4,y,z (m_z | 1/2,1/2,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity,  Coordinates
Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 j</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2)  x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3)  x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4)  x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5)  x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6)  x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7)  x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8)  x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 i</td>
<td>8</td>
<td>m' x,1/4,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3/4 x+1/2,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3/4 x+1/2,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/4 x+1/2,3/4 [u,v,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>8</td>
<td>m x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>8</td>
<td>2' x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 e</td>
<td>4</td>
<td>m' 0,1/4,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3/4,1/4,3/4 [u,0,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>4</td>
<td>2'/m' 1/4,1/4,3/4 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3/4,1/4,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>4</td>
<td>2'/m' 1/4,1/4,1/4 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3/4,1/4,1/4 [u,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>4</td>
<td>2/m' 0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>4</td>
<td>2/m' 0,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p2mm'  Along [1,0,0]  c2mm1'  Along [0,1,0]  c2mm'
\( a^* = a/2 \)  \( b^* = b/2 \)  \( a^* = b \)  \( b^* = c \)  \( a^* = -a \)  \( b^* = c \)
**Im'm'a'**

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**m'm'm'**

l2/m2/l'm2/a'

**Orthorhombic**

Origin at center (2/m') at 2/m'2,n'b'

**Symmetry Operations**

**Asymmetric unit**

\[0 < x < 1/4; \quad 0 < y < 1/4; \quad 0 < z < 1\]

**For (0,0,0) + set**

(1) \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)

(1) \( 0,0,0 \)

(2) \( 0,1/4,z \)

(2) \( 0,1/2,0 \)

(3) \( 0,1/2,0 \)

(4) \( x,0,0 \)

\( (2,m) \)

\( 0,0,0 \)

\( (2,z) \)

\( 0,0,0 \)

\( 0,0,0 \)

(5) \( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \)

(6) \( b', 0,1/2,0 \)

(6) \( m', 0,1/2,0 \)

\( y,x,0 \)

\( x,y,0 \)

\( y,x,0 \)

(7) \( m', 0,1/4,z \)

(7) \( m', 0,1/4,z \)

\( x,0,0 \)

\( 0,0,0 \)

\( 0,0,0 \)

\( 0,0,0 \)

\( 0,0,0 \)

\( 0,0,0 \)

**For (1/2,1/2,1/2) + set**

(1) \( 1/2,1/2,1/2 \)

(1) \( 1/2,1/2,1/2 \)

(1) \( 1/2,1/2,1/2 \)

(2) \( 0,0,1/2 \)

(2) \( 0,1/2,0 \)

(2) \( 1/2,1/2,1/2 \)

(2) \( 0,1/2,0 \)

(2) \( 1/2,1/2,1/2 \)

\( 1/4,0,z \)

\( 1/4,0,z \)

\( 1/4,0,z \)

\( 1/4,0,z \)

\( 1/4,0,z \)

\( 1/4,0,z \)

\( 1/4,0,z \)

(3) \( 1/4,y,1/4 \)

(3) \( 1/4,y,1/4 \)

(3) \( 1/4,y,1/4 \)

(3) \( 1/4,y,1/4 \)

(3) \( 1/4,y,1/4 \)

(3) \( 1/4,y,1/4 \)

(3) \( 1/4,y,1/4 \)

(4) \( 1/2,0,0 \)

(4) \( 1/2,0,0 \)

(4) \( 1/2,0,0 \)

(4) \( 1/2,0,0 \)

(4) \( 1/2,0,0 \)

(4) \( 1/2,0,0 \)

(4) \( 1/2,0,0 \)

For (1/2,1/2,1/2) + set

(1) \( 1/2,1/2,1/2 \)

(2) \( 1/2,1/2,1/2 \)

(2) \( 1/2,1/2,1/2 \)

(2) \( 1/2,1/2,1/2 \)

(2) \( 1/2,1/2,1/2 \)

(2) \( 1/2,1/2,1/2 \)

(2) \( 1/2,1/2,1/2 \)

(2) \( 1/2,1/2,1/2 \)

(3) \( 1/2,0,1/2 \)

(3) \( 1/2,0,1/2 \)

(3) \( 1/2,0,1/2 \)

(3) \( 1/2,0,1/2 \)

(3) \( 1/2,0,1/2 \)

(3) \( 1/2,0,1/2 \)

(3) \( 1/2,0,1/2 \)

(3) \( 1/2,0,1/2 \)

(4) \( 1/4,y,1/4 \)

(4) \( 1/4,y,1/4 \)

(4) \( 1/4,y,1/4 \)

(4) \( 1/4,y,1/4 \)

(4) \( 1/4,y,1/4 \)

(4) \( 1/4,y,1/4 \)

(4) \( 1/4,y,1/4 \)

(4) \( 1/4,y,1/4 \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>(2) x,y+1/2,z [u,v,0]</td>
<td>(3) x,y+1/2,z [u,v,0]</td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(6) x,y+1/2,z [u,v,w]</td>
<td>(7) x,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(8) x,y,z [u,v,w]</td>
<td>(9) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2m'm'  Along [1,0,0] c2m'm'  Along [0,1,0] c2m'm'

a* = a/2   b* = b/2
Origin at 0,0,z

Along [1,0,0] c2m'm'  Along [0,1,0] c2m'm'

a* = a   b* = c
Origin at x,1/4,1/4

Along [0,0,1] p2m'm'

a* = c   b* = a
Origin at 0,y,0

74.7.656 - 2 - 1305
IPmma

Orthorhombic

74.8.657

IPmma

Orthorhombic

74.8.657

mmm1'

I_{21/m21/m21/a}

Origin at center (2/m) at 2/m21/n'b

Asymmetric unit

0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) 1

(1 | 0,0,0)

(2) 2 0,1/4,z

(2 | 0,1/2,0)

(3) 2 (0,1/2,0) 0,y,0

(2 | 0,1/2,0)

(4) 2 x,0,0

(2 | 0,0,0)

(5) 1

(0,0,0)

(6) b (0,1/2,0) x,y,0

(m_0 | 0,1/2,0)

(7) m x,1/4,z

(0 | 0,0,0)

(8) m y,z

(0 | 0,0,0)

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)

(1/2 | 1/2,1/2,1/2)

(2) 2' (0,0,1/2) 1/4,0,z

(2 | 1/2,0,1/2)

(3) 2' 1/4,y,1/4

(2 | 1/2,0,1/2)

(4) 2' x,1/4,1/4

(2 | 1/2,1/2,1/2)

(5) t' (1/4,1/4,1/4)

(1/2 | 1/2,1/2,1/2)

(6) a' (1/2,0,0) x,y,1/4

(m_0 | 1/2,0,1/2)

(7) n' (1/2,0,1/2) x,0,z

(m_0 | 1/2,0,1/2)

(8) n' (0,1/2,1/2) 1/4,y,z

(m_0 | 1/2,1/2,1/2)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 j 1 (1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>(2) x,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(3) x,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 i .m. x,1/4,z [0,v,0]</td>
<td>x,1/4,z [0,v,0]</td>
</tr>
<tr>
<td>x,3/4,z [0,v,0]</td>
<td>x,3/4,z [0,v,0]</td>
</tr>
<tr>
<td>8 h m.. 0,y,z [u,0,0]</td>
<td>0,y+1/2,z [u,0,0]</td>
</tr>
<tr>
<td>0,y+1/2,z [0,v,0]</td>
<td>0,y+1/2,z [u,0,0]</td>
</tr>
<tr>
<td>0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 g .2'. 1/4,y,1/4 [u,0,w]</td>
<td>3/4,y+1/2,1/4 [u,0,w]</td>
</tr>
<tr>
<td>3/4,y+1/2,1/4 [u,0,w]</td>
<td>3/4,y+1/2,1/4 [u,0,w]</td>
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<tr>
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<td>1/4,y+1/2,3/4 [u,0,w]</td>
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<td>x,1/2,0 [u,0,0]</td>
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<tr>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
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<td>x,1/2,0 [u,0,0]</td>
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<tr>
<td>4 e mm2 0,1/4,z [0,0,0]</td>
<td>0,1/4,z [0,0,0]</td>
</tr>
<tr>
<td>4 d .2'/m. 1/4,1/4,3/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c .2'/m. 1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b 2/m.. 0,0,1/2 [u,0,0]</td>
<td>1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 a 2/m.. 0,0,0 [u,0,0]</td>
<td>0,1/2,0 [u,0,0]</td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [0,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p2\text{a}2mm</td>
<td>a* = -b/2</td>
<td>b* = a/2</td>
<td>c2mm1'</td>
</tr>
<tr>
<td>c2mm1'</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = c</td>
</tr>
<tr>
<td>Origin at 0,1/4,z</td>
<td>Origin at x,1/4,1/4</td>
<td>Origin at 0,y,0</td>
<td></td>
</tr>
</tbody>
</table>
Orthorhombic

$74.9.658$

$\text{mmm}1'$

$\text{l}_{2}'/\text{m}'2_/l_{2}'/\text{m}'2_/a$

**Origin** at center $(2'/{\text{m'}})$ at $2'/{\text{m'}2'/\text{m }'b}$

**Asymmetric unit**

$0 < x < 1/4; \quad 0 < y < 1/4; \quad 0 < z < 1$

**Symmetry Operations**

For $(0,0,0) +$ set

$(1) \ 1 \ (1 | 0,0,0)$

$(2) \ 2 \ (0,1/2,0) \ (2_z | 0,1/2,0)$

$(3) \ 2' \ (0,1/2,0) \ 0,y,0 \ (2_z | 0,1/2,0)'$

$(4) \ 2' \ x,0,0 \ (2_z | 0,0,0)'$

$(5) \ {\text{m'}} \ 0,0,0 \ (1 | 0,0,0)$

$(6) \ {\text{b}} \ (0,1/2,0) \ x,y,0 \ (m_z | 0,1/2,0)$

$(7) \ m' \ x,1/4,z \ (m_y | 0,1/2,0)'$

$(8) \ m' \ 0,y,z \ (m_z | 0,0,0)'$

For $(1/2,1/2,1/2)' +$ set

$(1) \ t' \ (1/2,1/2,1/2) \ (1 | 1/2,1/2,1/2)'$

$(2) \ 2' \ (0,0,1/2) \ 1/4,0,z \ (2_z | 1/2,0,1/2)'$

$(3) \ 2 \ 1/4,y,1/4 \ (2_y | 1/2,0,1/2)$

$(4) \ 2 \ (1/2,0,0) \ x,1/4,1/4 \ (2_x | 1/2,1/2,1/2)$

$(5) \ {\text{t'}} \ 1/4,1/4,1/4 \ (1 | 1/2,1/2,1/2)'$

$(6) \ a' \ (1/2,0,0) \ x,y,1/4 \ (m_z | 1/2,0,1/2)'$

$(7) \ n \ (1/2,0,1/2) \ x,0,z \ (m_y | 1/2,0,1/2)$

$(8) \ n \ (0,1/2,1/2) \ 1/4,y,z \ (m_z | 1/2,1/2,1/2)$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 j</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y+1/2, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+1/2, y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y+1/2, z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y+1/2, z [u,v,w]</td>
</tr>
<tr>
<td>8 i</td>
<td>x,1/4,z [u,0,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>8 g</td>
<td>1/4,y,1/4 [0,v,0]</td>
</tr>
<tr>
<td>8 f</td>
<td>0,0,0 [0,v,w]</td>
</tr>
<tr>
<td>4 e</td>
<td>0,1/4,z [0,0,w]</td>
</tr>
<tr>
<td>4 d</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  $p_{2a} \cdot 2m'm'$   
Along [1,0,0]  $c_p \cdot 2mm'$   
Along [0,1,0]  $c_p \cdot 2mm'$

$a^* = -b/2$  \hspace{1cm} $b^* = a/2$

Origin at 0,1/4,z   
Origin at x,1/4,1/4   
Origin at 0,y,0
Origin at center (2/m) at 2/m2,'h/n'b'

Asymmetric unit

\[ 0 < x < \frac{1}{4}; \quad 0 < y < \frac{1}{4}; \quad 0 < z < 1 \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) \ & 1 \\
(1) \ & (0,0,0) \\
(2) \ & 2', 0,1/4,z \\
(2) \ & (0,1/2,0)' \\
(3) \ & 2' (0,1/2,0) 0,y,0 \\
(3) \ & (2',0,1/2,0)' \\
(4) \ & 2 x,0,0 \\
(4) \ & (2,0,0,0) \\
(5) \ & 0,0,0 \\
(5) \ & (1,0,0,0) \\
(6) \ & b' (0,1/2,0) x,y,0 \\
(6) \ & (m_z,0,1/2,0)' \\
(7) \ & m' x,1/4,z \\
(7) \ & (m_y,0,1/2,0)' \\
(8) \ & m 0,y,z \\
(8) \ & (m,0,0,0) \\
\end{align*}
\]

For \((1/2,1/2,1/2)'\) + set

\[
\begin{align*}
(1) \ & t' (1/2,1/2,1/2) \\
(1) \ & (1/2,1/2,1/2)' \\
(2) \ & 2 (0,0,1/2) 1/4,0,z \\
(2) \ & (2,1/2,0,1/2) \\
(3) \ & 2 1/4,y,1/4 \\
(3) \ & (2,1/2,0,1/2) \\
(4) \ & 2' (1/2,0,0) x,1/4,1/4 \\
(4) \ & (2,1/2,1/2,1/2)' \\
(5) \ & 1/4,1/4,1/4 \\
(5) \ & (1/2,1/2,1/2)' \\
(6) \ & a (1/2,0,0) x,y,1/4 \\
(6) \ & (m_z,1/2,0,1/2) \\
(7) \ & n (1/2,0,1/2) x,0,z \\
(7) \ & (m_y,1/2,0,1/2) \\
(8) \ & n' (0,1/2,1/2) 1/4,y,z \\
(8) \ & (m,1/2,1/2,1/2)' \\
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 j</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y+1/2,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2)' + (u,v,w)</td>
</tr>
<tr>
<td>8 i</td>
<td>.m'</td>
<td>(5) x,y,z [u,v,w]</td>
<td>(u,v,w)</td>
</tr>
<tr>
<td>8 h</td>
<td>m..</td>
<td>(6) x,y+1/2,z [u,v,w]</td>
<td>(u,v,w)</td>
</tr>
<tr>
<td>8 g</td>
<td>.2.</td>
<td>(7) x,y+1/2,z [u,v,w]</td>
<td>(u,v,w)</td>
</tr>
<tr>
<td>8 f</td>
<td>2..</td>
<td>(8) x,y,z [u,v,w]</td>
<td>(u,v,w)</td>
</tr>
<tr>
<td>4 e</td>
<td>mm'2'</td>
<td>0,1/4,z [u,0,0]</td>
<td>0,3/4,z [u,0,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>.2/m'.</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>.2/m'.</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>2/m..</td>
<td>0,1/2,1/2 [u,0,0]</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>2/m..</td>
<td>0,0,0 [u,0,0]</td>
<td>0,1/2,0 [u,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p2mm'
  - $a^* = a/2$, $b^* = b/2$
  - Origin at 0,0,z

- Along [1,0,0] c2mm1'
  - $a^* = b$, $b^* = c$
  - Origin at x,1/4,1/4

- Along [0,1,0] $c_p$-2mm'
  - $a^* = -a$, $b^* = c$
  - Origin at 0,y,0
Orthorhombic

74.11.660

Orthorhombic

I_p'm'ma'

mm1'

I_p2,1/m'/2,m2,1/a'

Origin at center (2'/m') at 2'/m'2,1/b'

Asymmetric unit

0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2' 0,1/4,z
    (2 | 0,1/2,0)

(3) 2 (0,1/2,0) 0,y,0
    (2 | 0,1/2,0)

(4) 2' x,0,0
    (2 | 0,0,0)

(5) 1/m
    (1 | 0,0,0)

(6) b' (0,1/2,0) x,y,0
    (m | 0,1/2,0)

(7) m x,1/4,z
    (m | 0,1/2,0)

(8) m' 0,y,z
    (m | 0,0,0)

For (1/2,1/2,1/2)′ + set

(1) t' (1/2,1/2,1/2)
    (1 | 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,0,z
    (2 | 1/2,0,1/2)

(3) 2' 1/4,y,1/4
    (2 | 1/2,0,1/2)

(4) 2 (1/2,0,0) x,1/4,1/4
    (2 | 1/2,1/2,1/2)

(5) 1/m'
    (1 | 1/2,1/2,1/2)

(6) a (1/2,0,0) x,y,1/4
    (m | 1/2,0,1/2)

(7) n' (1/2,0,1/2) x,0,z
    (m | 1/2,0,1/2)

(8) n (0,1/2,1/2) 1/4,y,z
    (m | 1/2,1/2,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2) x,y+1/2,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3) x,y+1/2,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(6) x,y+1/2,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7) x,y+1/2,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(8) x,y,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(2) x,y+1/2,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3) x,y+1/2,z [u,v,w]</td>
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<td></td>
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<tr>
<td>(4) x,y,z [u,v,w]</td>
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<td></td>
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<tr>
<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td>(2) x,y+1/2,z [u,v,w]</td>
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<td></td>
</tr>
<tr>
<td>(3) x,y+1/2,z [u,v,w]</td>
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<td></td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Along [0,0,1] p2mm'</th>
<th>Along [1,0,0] c_p 2mm</th>
<th>Along [0,1,0] c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = -b/2 b^* = a/2</td>
<td>a^* = b b^* = c</td>
<td>a^* = c b^* = a</td>
<td>a^* = c b^* = a</td>
</tr>
</tbody>
</table>

74.11.660 - 2 - 1313
Origin on 4

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

(1) 1
(1)|0,0,0)

(2) 2 0,0,z
(2z)|0,0,0)

(3) 4z 0,0,z
(4z)|0,0,0)

(4) 4z -1 0,0,z
(4z) -1|0,0,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>2 c 2</td>
<td>0,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>1 b 4</td>
<td>1/2,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>1 a 4</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4</th>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = (a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 41'

Asymmetric unit \(0 \leq x \leq 1/2;\) \(0 \leq y \leq 1/2;\) \(0 \leq z \leq 1\)

Symmetry Operations

For 1 + set

\[(1) 1 (2) 2 0,0,z (3) 4^+ 0,0,z (4) 4^- 0,0,z \]

\[(1^* 0,0,0) (2^z 0,0,0) (4^z 0,0,0) (4^z^{-1} 0,0,0)\]

For 1' + set

\[(1) 1' (2) 2' 0,0,z (3) 4'^+ 0,0,z (4) 4'^- 0,0,z \]

\[(1^* 0,0,0)' (2^z 0,0,0)' (4^z 0,0,0)' (4^z^{-1} 0,0,0)'\]
Continued

75.2.662

P41'

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

**Positions**

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>+</td>
<td></td>
</tr>
<tr>
<td>1'</td>
<td>+</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>d</th>
<th>11'</th>
<th>(1) x,y,z [0,0,0]</th>
<th>(2) x̅,y,z [0,0,0]</th>
<th>(3) y,x,z [0,0,0]</th>
<th>(4) y,x̅,z [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>c</td>
<td>2..1'</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>4..1'</td>
<td>1/2,1/2,z [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>4..1'</td>
<td>0,0,z [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p41'

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

Along [1,0,0] p1m11'

\[ a^* = b \quad b^* = c \]

Origin at x,0,0

Along [1,1,0] p1m11'

\[ a^* = (a + b)/2 \quad b^* = c \]

Origin at x,x,0
Origin on 4'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

(1) 1
(2) 2 0,0,z
(3) $4'$ 0,0,z
(4) $4'$ 0,0,z

$1\,(0,0,0)
2\,(z,0,0,0)
3\,(4z,0,0,0)
4\,(4z,0,0,0')$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>2 c 2..</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>1 b 4'..</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>1 a 4'..</td>
<td>0,0,z [0,0,0]</td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'</th>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 4

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

(1) $1$
(2) $2 \cdot 0,0,z$
(3) $4^+ \cdot 0,0,z$
(4) $4^- \cdot 0,0,z$

For $(0,0,1)'$ + set

(1) $t\cdot (0,0,1)$
(2) $2' \cdot (0,0,1) \cdot 0,0,z$
(3) $4'^+ \cdot (0,0,1) \cdot 0,0,z$
(4) $4'^- \cdot (0,0,1) \cdot 0,0,z$

P$_{2c}$ 4

Tetragonal

75.4.664 - 1 - 1320
Generators selected \( \text{t}(1,0,0); \text{t}(0,1,0); \text{t}(0,0,1)^*; \text{t}; (2); (3). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
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<tbody>
<tr>
<td>( 8 ) d 1</td>
<td>((0,0,0) + (0,0,1)^* + )</td>
</tr>
<tr>
<td>( 4 ) c 2..</td>
<td>((0,0,1))</td>
</tr>
<tr>
<td>( 2 ) b 4..</td>
<td>((0,0,1))</td>
</tr>
<tr>
<td>( 2 ) a 4..</td>
<td>((0,0,1))</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along ([0,0,1])</th>
<th>(p41^*)</th>
<th>Along ([1,0,0])</th>
<th>(p_{2b}1m1)</th>
<th>Along ([1,1,0])</th>
<th>(p_{2b}1m1)</th>
</tr>
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<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = b)</td>
<td>(b^* = c)</td>
<td>(a^* = (-a + b)/2)</td>
<td>(b^* = c)</td>
</tr>
</tbody>
</table>
Origin on 4

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 0,0,z \\
(2) & \quad (0,0,0) \\
(3) & \quad 4^+ \quad 0,0,z \\
(3) & \quad (4z|0,0,0) \\
(4) & \quad 4^- \quad 0,0,z \\
(4) & \quad (4z^{-1}|0,0,0)
\end{align*}
\]

For \((1,0,0)'\) + set

\[
\begin{align*}
(1) & \quad t' \quad (1,0,0) \\
(1) & \quad (1,0,0)' \\
(2) & \quad 2' \quad 1/2,0,z \\
(2) & \quad (2z|1,0,0)' \\
(3) & \quad 4^+ \quad 1/2,1/2,z \\
(3) & \quad (4z|1,0,0)' \\
(4) & \quad 4^- \quad 1/2,1/2,z \\
(4) & \quad (4z^{-1}|1,0,0)'
\end{align*}
\]
### Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

### Positions

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<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 c 2'..</td>
<td>0,1/2,z [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>2 b 4'..</td>
<td>1/2,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1], \( p_p 4 \)

- \( \mathbf{a}^* = \mathbf{a} \)
- \( \mathbf{b}^* = \mathbf{b} \)
- Origin at 0,0,z

Along [1,0,0], \( p1m11' \)

- \( \mathbf{a}^* = \mathbf{b} \)
- \( \mathbf{b}^* = \mathbf{c} \)
- Origin at x,0,0

Along [1,1,0], \( p_{221} 1m1 \)

- \( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \)
- \( \mathbf{b}^* = \mathbf{c} \)
- Origin at x-1/4,x+1/4,0
Origin on 4

Asymmetric unit  \[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0) + \) set

(1) 1
(1|0,0,0)

(2) 2 \(\times \) 0,0,z
(2|0,0,0)

(3) 4^+ \(\times \) 0,0,z
(4|z|0,0,0)

(4) 4^- \(\times \) 0,0,z
(4|z^-1|0,0,0)

For \((1,0,0) + \) set

(1) t' \(\times \) (1,0,0)
(1|1,0,0)

(2) 2' \(\times \) 1/2,0,z
(2|z|1,0,0)

(3) 4^+ \(\times \) 1/2,1/2,z
(4|z|1,0,0)

(4) 4^- \(\times \) 1/2,1/2,z
(4|z^-1|1,0,0)
Generators selected (1); \(t'(1,0,0); t'(0,1,0); t'(0,0,1)\); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>((0,0,0) + (1,0,0)' + (0,1,0)' + (0,0,1))</td>
</tr>
<tr>
<td>4 c 2'..</td>
<td>((0,1/2,z) [u,v,0] 1/2,0,z [v,u,0] )</td>
</tr>
<tr>
<td>2 b 4'..</td>
<td>((1/2,1/2,z) [0,0,0] )</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>((0,0,z) [0,0,w] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \(p41'\) \(a^* = a \quad b^* = b\)
Origin at 0,0,z

Along \([1,0,0]\) \(p1m1'\) \(a^* = b \quad b^* = c\)
Origin at x,0,0

Along \([1,1,0]\) \(p_{1c}1m1\) \(a^* = (-a + b)/2 \quad b^* = c\)
Origin at x-1/4,x+1/4,0
Origin on 4

Asymmetric unit \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0) + \text{set}\)

\begin{align*}
(1) & \text{1} \\
(1|0,0,0) & \\
(2) & 0,0,z \\
(2_2|0,0,0) & \\
(3) & 4^* 0,0,z \\
(4_z|0,0,0)' & \\
(4) & 4^* 0,0,z \\
(4_z^{-1}|0,0,0)' &
\end{align*}

For \((0,0,1)' + \text{set}\)

\begin{align*}
(1) & t' (0,0,1) \\
(1|0,0,1)' & \\
(2) & 2' (0,0,1) 0,0,z \\
(2_z|0,0,1)' & \\
(3) & 4^* (0,0,1) 0,0,z \\
(4_z|0,0,1) & \\
(4) & 4^* (0,0,1) 0,0,z \\
(4_z^{-1}|0,0,1) &
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1)'; (2); (3).

Positions

Multiplicity,  Coordinates
Wyckoff letter, (0,0,0) + (0,0,1) +
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c 2..</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 b 4..</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p41'  Along [1,0,0]  p21m1  Along [1,1,0]  p21m1
\( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)  \( \mathbf{a}^* = \mathbf{b} \)  \( \mathbf{b}^* = \mathbf{c} \)
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0  Origin at x,x,0

\( \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \)  \( \mathbf{b}^* = \mathbf{c} \)
Origin on 4₁

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)

Symmetry Operations

(1) 1
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2|0,0,1/2)

(3) 4⁺ (0,0,1/4) 0,0,z
(4|0,0,1/4)

(4) 4⁻ (0,0,3/4) 0,0,z
(4⁻|0,0,3/4)
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

**Positions**

- **Multiplicity**
- **Wyckoff letter**
- **Site Symmetry**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 a 1</td>
<td>((1) \ x, y, z \ [u, v, w])</td>
</tr>
<tr>
<td></td>
<td>((2) \ \bar{x}, \bar{y}, \bar{z} + 1/2 \ [\bar{u}, \bar{v}, w])</td>
</tr>
<tr>
<td></td>
<td>((3) \ y, x, z + 1/4 \ [v, u, w])</td>
</tr>
<tr>
<td></td>
<td>((4) \ y, x, z + 3/4 \ [v, u, w])</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along \([0,0,1]\) p4**
- **Along \([1,0,0]\) p1g'1**
- **Along \([1,1,0]\) p1g'1**

\( a^* = a \quad b^* = b \)
\( a^* = b \quad b^* = c \)
\( a^* = (-a + b)/2 \quad b^* = c \)

Origin at \((0,0,0)\)  Origin at \((x,0,0)\)  Origin at \((x,x,0)\)
Origin on 4,1'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For 1 + set

(1) 1
(1' 0,0,0)
(2) 2 (0,0,1/2) 0,0,z
(2' 0,0,1/2')
(3) 4+ (0,0,1/4) 0,0,z
(4z 0,0,1/4)
(4z' 0,0,3/4)

For 1' + set

(1) 1'
(1' 0,0,0')
(2) 2' (0,0,1/2) 0,0,z
(2' 0,0,1/2')
(3) 4' (0,0,1/4) 0,0,z
(4z' 0,0,1/4')
(4z' 0,0,3/4')
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 +</td>
<td>1' +</td>
</tr>
<tr>
<td>4 a 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x̅,y̅,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y̅,x̅,z+1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x̅,z+3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p41'</th>
<th>Along [1,0,0]</th>
<th>p1g11'</th>
<th>Along [1,1,0]</th>
<th>p1g11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on $4_{1}^{'},$

Asymmetric unit  

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

1. 1
   
2. 2 $\{0,0,1/2\}$ 0,0,z
   
3. $4_{1}^{'},$ 0,0,$1/4$ 0,0,z
   
4. $4_{1}^{'},$ 0,0,$3/4$ 0,0,z
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

4  a  1  (1) x,y,z [u,v,w]  (2) x,y,z+1/2 [u,v,w]  (3) y,x,z+1/4 [v,u,w]  (4) y,x,z+3/4 [v,u,w]

Symmetry of Special Projections

Along [0,0,1]  p4'  Along [1,0,0]  p1g'1  Along [1,1,0]  p1g'1
a* = a  b* = b  a* = b  b* = c  a* = (a + b)/2  b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
Origin on 41

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad \text{1} \\
(2) & \quad \text{2} (0,0,1/2) \quad 0,0,z \\
(3) & \quad \text{4}^+ (0,0,1/4) \quad 0,0,z \\
(4) & \quad \text{4}^- (0,0,3/4) \quad 0,0,z
\end{align*}
\]

For \((1,0,0)\) + set

\[
\begin{align*}
(1) & \quad \text{1} (1,0,0) \\
(2) & \quad \text{2} (0,0,1/2) \quad 1/2,0,z \\
(3) & \quad \text{4}^+ (0,0,1/4) \quad 1/2,1/2,z \\
(4) & \quad \text{4}^- (0,0,3/4) \quad 1/2,1/2,z
\end{align*}
\]
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 a 1</td>
<td>(1) x,y,z [u,v,w] (2) x̄,ȳ,z+1/2 [u̅,v̅,w̅] (3) ȳ̄,x̄,z+1/4 [v̅,u̅,w̅] (4) y̅,x̅,z+3/4 [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] pₚ 4</th>
<th>Along [1,0,0] p₁g 11'</th>
<th>Along [1,1,0] p₂a 1g 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = (-a + b)/2 b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x-1/4,x+1/4,0</td>
</tr>
</tbody>
</table>
Origin on 2 on 42

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

1. \(1\)  
   \((1|0,0,0)\)

2. \(2\)
   \((0,0,z)\)

3. \(4^+ (0,0,1/2)\)
   \((0,0,z)\)

4. \(4^- (0,0,1/2)\)
   \((0,0,z)\)

\((4_z |0,0,1/2)\)
\((4_z^{-1} |0,0,1/2)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>p4</td>
</tr>
<tr>
<td>2</td>
<td>c 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 2..</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a 2..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4  
Along [1,0,0] p1m'1  
Along [1,1,0] p1m'1

a* = a  
b* = b

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0
Origin on 21' on 421'

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\]

Symmetry Operations

For 1 + set

1. \(1 \quad (1|0,0,0)\)
2. \(2' \quad 0,0,z \quad (2_z|0,0,0)\)
3. \(4' \quad (0,0,1/2) \quad 0,0,z \quad (4_z|0,0,1/2)\)
4. \(4' \quad (0,0,1/2) \quad 0,0,z \quad (4_z^{-1}|0,0,1/2)\)

For 1' + set

1. \(1' \quad (1|0,0,0)'\)
2. \(2' \quad 0,0,z \quad (2_z|0,0,0)'\)
3. \(4' \quad (0,0,1/2) \quad 0,0,z \quad (4_z|0,0,1/2)'\)
4. \(4' \quad (0,0,1/2) \quad 0,0,z \quad (4_z^{-1}|0,0,1/2)'\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>1</th>
<th>1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>(3) x, y, z+1/2 [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>(4) y, x, z+1/2 [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td>2 c 2.1'</td>
<td>0,1/2, z [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>1/2,0, z+1/2 [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td>2 b 2.1'</td>
<td>1/2, 1/2, z [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>1/2, 1/2, z+1/2 [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td>2 a 2.1'</td>
<td>0,0, z [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>0,0, z+1/2 [0,0,0]</td>
<td>1</td>
<td>1'</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'  
\[ a^* = a, \ b^* = b \]
Origin at 0,0,z

Along [1,0,0] p1m11'  
\[ a^* = b, \ b^* = c \]
Origin at x,0,0

Along [1,1,0] p1m11'  
\[ a^* = (-a + b)/2, \ b^* = c \]
Origin at x,x,0
**Origin** on 2 on $4'_z$

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 2 \\
(2_z) & \quad (0,0,0) \\
(3) & \quad 4'_z \cdot (0,0,1/2) \\
(4_z) & \quad 0,0,0 \\
(4'_z) & \quad (0,0,1/2) \\
(4_z^{-1}) & \quad (0,0,1/2) \\
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions  
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>4</th>
<th>d</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) y,x,z+1/2 [v,u,w]</th>
<th>(4) y,x,z+1/2 [v,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>c</td>
<td>2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>2..</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>2..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1]  p4  
\(a^* = a\)  \(b^* = b\)  Origin at 0,0,z
Along [1,0,0]  p1m'1  \(a^* = b\)  \(b^* = c\)  Origin at x,0,0
Along [1,1,0]  p1m'1  \(a^* = (-a + b)/2\)  \(b^* = c\)  Origin at x,x,0
Origin on $2'$ on $4_2$

Asymmetric unit \[0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1\]

Symmetry Operations

For $(0,0,0)$ +

1. $1$
2. $2'$ \((0,0,z)\)
3. $4^+ (0,0,1/2) \quad 0,0,z$
4. $4^- (0,0,1/2) \quad 0,0,z$

For $(0,0,1)'$ +

1. $(0,0,1)'$
2. $2 \quad (0,0,1) \quad 0,0,z$
3. $4^+ (0,0,3/2) \quad 0,0,z$
4. $4^- (0,0,3/2) \quad 0,0,z$
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) $x, y, z$ [u, v, w]</td>
</tr>
<tr>
<td>4 c 2</td>
<td>0,1/2,$z$ [0,0,$w$]</td>
</tr>
<tr>
<td>4 b 2</td>
<td>1/2,1/2,$z$ [0,0,$w$]</td>
</tr>
<tr>
<td>4 a 2</td>
<td>0,0,$z$ [0,0,$w$]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4       Along [1,0,0] p1m1       Along [1,1,0] p1m1
\(a^* = a\) \(b^* = b\) \(a^* = b\) \(b^* = c\) \(a^* = (-a + b)/2\) \(b^* = c\)
Origin at 0,0,$z$       Origin at $x,0,0$       Origin at $x,x,0$
Origin on 2 on 42

Asymmetric unit

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1\]

Symmetry Operations

For \((0,0,0)\) + set

\[(1) 1
(2) 2 \quad 0,0,z
(3) 4^+ (0,0,1/2) \quad 0,0,z
(4) 4^- (0,0,1/2) \quad 0,0,z\]

For \((1,0,0)'\) + set

\[(1)' (1,0,0)
(2)' 2' \quad 1/2,0,z
(3)' 4^+ ' (0,0,1/2) \quad 1/2,1/2,z
(4)' 4^- ' (0,0,1/2) \quad 1/2,1/2,z\]

77.5.676 - 1 - 1344
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1,0,0)' +</td>
<td></td>
</tr>
<tr>
<td>8  d  1 (1) x,y,z [u,v,w] (2) (\bar{x},\bar{y},\bar{z}) [(\bar{u},\bar{v},\bar{w})] (3) (\bar{y},x,z+1/2) [(\bar{v},u,w)] (4) (y,\bar{x},z+1/2) [(v,\bar{u},w)]</td>
<td></td>
</tr>
<tr>
<td>4  c  2'.. 0,1/2,z [u,v,0] 1/2,0,z+1/2 [v,(\bar{u}),0]</td>
<td></td>
</tr>
<tr>
<td>4  b  2.. 1/2,1/2,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4  a  2.. 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p2(\times)4</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [1,1,0]</th>
<th>p2(\times)1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = b)</td>
<td>(b^* = c)</td>
<td>(a^* = (-a+b)/2)</td>
<td>(b^* = c)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x-1/4,x+1/4,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2' on 4₂

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \]

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
2. \((1',0,0)\)
3. \((2',0,0,0)'\)

\((1,0,0)\) + set

1. \((1,0,0)\)
2. \((1,1,0,0)\)
3. \((2,0,0,0)\)

\((2,0,0,0)\) + set

1. \((1,0,0,0)\)
2. \((1,1,0,0)\)
3. \((2,0,0,0)\)
4. \((2,0,0,0)\)
Generators selected \( (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>((0,0,0) + (1,0,0)' + )</td>
<td>((0,0,0) + (1,0,0)' + )</td>
</tr>
<tr>
<td>4 c 2..</td>
<td>(0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] )</td>
<td>(0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] )</td>
</tr>
<tr>
<td>4 b 2'.</td>
<td>(1/2,1/2,z [u,v,0] 1/2,1/2,z+1/2 [v,u,0] )</td>
<td>(1/2,1/2,z [u,v,0] 1/2,1/2,z+1/2 [v,u,0] )</td>
</tr>
<tr>
<td>4 a 2'.</td>
<td>(0,0,z [u,v,0] 0,0,z+1/2 [v,u,0] )</td>
<td>(0,0,z [u,v,0] 0,0,z+1/2 [v,u,0] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

| Along [0,0,1] p41' | Along [1,0,0] p1m11' | Along [1,1,0] p\(\_
\_\_\_\_\)1m1 |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a \quad b^* = b)</td>
<td>(a^* = b \quad b^* = c)</td>
<td>(a^* = (-a + b)/2 \quad b^* = c)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 2' on 4'_z.

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)^+$

1. $1$
2. $2'$ $0,0,z$
3. $4^+ \cdot (0,0,1/2)$ $0,0,z$
4. $4^{-1} \cdot (0,0,1/2)$ $0,0,z$

For $(0,0,1)^+$

1. $1' (0,0,1)$
2. $2 (0,0,1) 0,0,z$
3. $4^+ \cdot (0,0,3/2) 0,0,z$
4. $4^{-1} \cdot (0,0,3/2) 0,0,z$
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (0,0,1)′ +</td>
</tr>
<tr>
<td>8 d 1 (1) x,y,z [u,v,w]</td>
<td>(2) x, y ,z [u,v,w]</td>
</tr>
<tr>
<td>4 c 2′.. 0,1/2,z [u,v,0]</td>
<td>1/2,0,z+1/2 [v,u,0]</td>
</tr>
<tr>
<td>4 b 2′.. 1/2,1/2,z [u,v,0]</td>
<td>1/2,1/2,z+1/2 [v,u,0]</td>
</tr>
<tr>
<td>4 a 2′.. 0,0,z [u,v,0]</td>
<td>0,0,z+1/2 [v,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p41′</th>
<th>Along [1,0,0] p2b1m1</th>
<th>Along [1,1,0] p2b1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = (a + b)/2 b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 4<sub>3</sub>

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations:

(1) 1
(1 | 0,0,0)

(2) 2 (0.0,1/2) 0.0,z
(2z | 0.0,1/2)

(3) 4<sup>+</sup> (0.0,3/4) 0.0,z
(4z | 0.0,3/4)

(4) 4<sup>-</sup> (0.0,1/4) 0.0,z
(4z<sup>-1</sup> | 0.0,1/4)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>a 1</td>
</tr>
</tbody>
</table>

(1) x,y,z [u,v,w]  
(2) x,y,z+1/2 [u,v,w]  
(3) y,x,z+3/4 [v,u,w]  
(4) y,x,z+1/4 [v,u,w]

Symmetry of Special Projections

Along [0,0,1]  p4  
Along [1,0,0]  p1g'1  
Along [1,1,0]  p1g'1

\[ a^* = a \quad b^* = b \]  
\[ a^* = b \quad b^* = c \]  
\[ a^* = (-a + b)/2 \quad b^* = c \]

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0
Origin on 4_3 1'  

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1  

Symmetry Operations  
For 1 + set  
(1) 1  
(1) 0,0,0  
(2) 2 (0,0,1/2) 0,0,z  
(2) 0,0,1/2  
(3) 4' (0,0,3/4) 0,0,z  
(3) 4'_1 0,0,3/4  
(4) 4' (0,0,1/4) 0,0,z  
(4) 4'_1 0,0,1/4  

For 1' + set  
(1) 1'  
(1) 0,0,0'  
(2) 2' (0,0,1/2) 0,0,z  
(2) 0,0,1/2'  
(3) 4'' (0,0,3/4) 0,0,z  
(3) 4''_1 0,0,3/4'  
(4) 4'' (0,0,1/4) 0,0,z  
(4) 4''_1 0,0,1/4')
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

Positions
Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
<td></td>
</tr>
<tr>
<td>4 a 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x̅,y̅,z̅+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y̅,x̅,z̅+3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) y̅,x̅,z̅+1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] p41'

<table>
<thead>
<tr>
<th>a* = a</th>
<th>b* = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>ab * = c</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

Along [1,0,0] p1g11'

<table>
<thead>
<tr>
<th>a* = b</th>
<th>b* = c</th>
</tr>
</thead>
<tbody>
<tr>
<td>a = (a + b)/2</td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

Along [1,1,0] p1g11'

<table>
<thead>
<tr>
<th>a* = (-a + b)/2</th>
<th>b* = c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 4_3'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

\begin{align*}
(1) \ 1 \\
(1 | 0,0,0) \\
(2) \ 2 \ (0,0,1/2) \ 0,0,z \\
(2_z | 0,0,1/2) \\
(3) \ 4' \ (0,0,3/4) \ 0,0,z \\
(4_z | 0,0,3/4') \\
(4) \ 4' \ (0,0,1/4) \ 0,0,z \\
(4_z^{-1} | 0,0,1/4')
\end{align*}
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>a 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x',y',z+1/2 [u',v',w']</td>
</tr>
<tr>
<td></td>
<td>(3) y',x,z+3/4 [v',u',w']</td>
</tr>
<tr>
<td></td>
<td>(4) y',x',z+1/4 [v',u',w']</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'  
Origin at 0,0,z  
$a^* = a$  
b* = b

Along [1,0,0] p1g'1  
Origin at x,0,0  
$a^* = b$  
b* = c

Along [1,1,0] p1g'1  
Origin at x,x,0  
a^* = (-a + b)/2  
b* = c
Origin on 4₃

Asymmetric unit  \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \) set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1) 1)</td>
<td>((1</td>
<td>0,0,0))</td>
</tr>
<tr>
<td>((2) 2)</td>
<td>((0,0,1/2))</td>
<td>(2z</td>
</tr>
<tr>
<td>((3) 4^*)</td>
<td>((0,0,3/4))</td>
<td>(4z</td>
</tr>
<tr>
<td>((4) 4^-)</td>
<td>((0,0,1/4))</td>
<td>(4z^{-1}</td>
</tr>
</tbody>
</table>

For \((1,0,0)' + \) set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1)')</td>
<td>((1,0,0))</td>
<td>(1,0,0)</td>
</tr>
<tr>
<td>((2)')</td>
<td>((0,0,1/2))</td>
<td>(2z</td>
</tr>
<tr>
<td>((3)')</td>
<td>((0,0,3/4))</td>
<td>(4z</td>
</tr>
<tr>
<td>((4)')</td>
<td>((0,0,1/4))</td>
<td>(4z^{-1}</td>
</tr>
</tbody>
</table>

\[78.4.682 - 1 - 1356\]
Generators selected \( (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 a 1</td>
<td>(1) ( x,y,z[u,v,w] ) (2) ( x,y,z+1/2[u,v,w] ) (3) ( y,x,z+3/4[v,u,w] ) (4) ( y,x,z+1/4[v,u,w] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4</th>
<th>Along [1,0,0] p1g'1</th>
<th>Along [1,1,0] p1g'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) ( b^* = b )</td>
<td>( a^* = b ) ( b^* = c )</td>
<td>( a^* = (-a + b)/2 ) ( b^* = c )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 4

Asymmetric unit \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0)\) + set

\((1)\) 1  
\((1|0,0,0)\)

\((2)\) 2 0,0,z  
\((2_z|0,0,0)\)

\((3)\) 4' 0,0,z  
\((4_z|0,0,0)\)

\((4)\) 4' 0,0,z  
\((4_z^{-1}|0,0,0)\)

For \((1/2,1/2,1/2)\) + set

\((1)\) t \((1/2,1/2,1/2)\)  
\((1|1/2,1/2,1/2)\)

\((2)\) 2 \((0,0,1/2)\) 1/4,1/4,z  
\((2_z|1/2,1/2,1/2)\)

\((3)\) 4' \((0,0,1/2)\) 0,1/2,z  
\((4_z|1/2,1/2,1/2)\)

\((4)\) 4' \((0,0,1/2)\) 1/2,0,z  
\((4_z^{-1}|1/2,1/2,1/2)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>4 b 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4  
\( \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \) \( \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \)  
Origin at 0,0,z

Along [1,0,0] c1m'1  
\( \mathbf{a}^* = \mathbf{b} \) \( \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [1,1,0] p1m'1  
\( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \) \( \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at x,x,0
Origin on 41'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $(0,0,0)$ + set

(1) $1$
   (1 | 0,0,0)

(2) $2 \cdot 0,0,z$
   (2 | 0,0,0)

(3) $4^+ \cdot 0,0,z$
   (4 | 0,0,0)

(4) $4^- \cdot 0,0,z$
   (4 | 0,0,0)

For $(1/2,1/2,1/2)$ + set

(1) $t (1/2,1/2,1/2)$
   (1 | 1/2,1/2,1/2)

(2) $2 \cdot (0,0,1/2)$
   (2 | 1/2,1/2,1/2)

(3) $4^+ (0,0,1/2) \cdot 0,1/2,z$
   (4 | 1/2,1/2,1/2)

(4) $4^- (0,0,1/2) \cdot 1/2,0,z$
   (4 | 1/2,1/2,1/2)

For $(0,0,0)' + set$

(1) $1'$
   (1 | 0,0,0)'

(2) $2' \cdot 0,0,z$
   (2 | 0,0,0)'

(3) $4^+ ' \cdot 0,0,z$
   (4 | 0,0,0)'

(4) $4^- ' \cdot 0,0,z$
   (4 | 0,0,0)'

For $(1/2,1/2,1/2)' + set$

(1) $t' (1/2,1/2,1/2)$
   (1 | 1/2,1/2,1/2)'

(2) $2' (0,0,1/2) \cdot 1/4,1/4,z$
   (2 | 1/2,1/2,1/2)'

(3) $4^+ ' (0,0,1/2) \cdot 0,1/2,z$
   (4 | 1/2,1/2,1/2)'

(4) $4^- ' (0,0,1/2) \cdot 1/2,0,z$
   (4 | 1/2,1/2,1/2)'

79.2.684 - 1 - 1360
Continued

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
<tr>
<td>8  c  11' (1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4  b  2..1' 0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2  a  4..1' 0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'  a* = (a - b)/2  b* = (a + b)/2  Origin at 0,0,z
Along [1,0,0] c1m11'  a* = b  b* = c  Origin at x,0,0
Along [1,1,0] p1m11'  a* = (-a + b)/2  b* = c/2  Origin at x,x,0
Origin on 4'

Asymmetric unit
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\]

Symmetry Operations

For \((0,0,0) + \text{ set}\):

1. \(1\)
   \[(1|0,0,0)\]

2. \(2\)
   \[(0,0,z)\]
   \[(2_z|0,0,0)\]

3. \(4^+\) \(0,0,z\)
   \[(4_z|0,0,0)\]

4. \(4^-\) \(0,0,z\)
   \[(4_z^{-1}|0,0,0)\]

For \((1/2,1/2,1/2) + \text{ set}\):

1. \(t\)
   \[(1/2,1/2,1/2,1/2)\]
   \[(1|1/2,1/2,1/2)\]

2. \(2\)
   \[(0,0,1/2)\]
   \[(1/2,1/2,1/2,1/2)\]

3. \(4^+\) \(0,0,1/2\)
   \[(4_z|1/2,1/2,1/2)\]

4. \(4^-\) \(0,0,1/2\)
   \[(4_z^{-1}|1/2,1/2,1/2)\]

79.3.685 - 1 - 1362
Continued 79.3.685 l4' 

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 b 2..</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a 4'..</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Origin at x,0,0</th>
<th>Origin at x,x,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2  b* = (a + b)/2</td>
<td>a* = b  b* = c</td>
<td>a* = (-a + b)/2  b* = c/2</td>
</tr>
</tbody>
</table>

Along [0,0,1] p4' Along [1,0,0] c1m'1 Along [1,1,0] p1m'1
Origin on 4

Asymmetric unit  
\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1\]

Symmetry Operations

For \((0,0,0) + \) set

1. \((1,0,0,0)\)
2. \((2,0,0,z)\)
3. \((4^+,0,0,z)\)
4. \((4^-0,0,z)\)

For \((1/2,1/2,1/2)' + \) set

1. \((1/2,1/2,1/2)\)
2. \((2',0,0,1/2)\)
3. \((4^+,0,0,1/2)\)
4. \((4^-0,0,1/2)\)

\((1/2,1/2,1/2)'\)

\((2_z1/2,1/2,1/2)'\)

\((4_z1/2,1/2,1/2)'\)
Generators selected  
(1): t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>c 1</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>4</td>
<td>b 2.</td>
<td>(0,1/2,0) [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a 4.</td>
<td>(0,0,0) [0,0,w] 2 a</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p_p 4  
\( \mathbf{a}^* = (a - b)/2 \)  \( \mathbf{b}^* = (a + b)/2 \)  
Origin at 0,0,z

Along [1,0,0]  c_p 1m'1  
\( \mathbf{a}^* = \mathbf{b} \)  \( \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [1,1,0]  p_2b 1m'1  
\( \mathbf{a}^* = (-a + b)/2 \)  \( \mathbf{b}^* = c/2 \)  
Origin at x,x,0
Origin on 4'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2z | 0,0,0)

(3) 4+ 0,0,z
(4z | 0,0,0)'

(4) 4− 0,0,z
(4z−1 | 0,0,0)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)'

(2) 2' (0,0,1/2) 1/4,1/4,z
(2z | 1/2,1/2,1/2)'

(3) 4+ (0,0,1/2) 0,1/2,z
(4z | 1/2,1/2,1/2)

(4) 4− (0,0,1/2) 1/2,0,z
(4z−1 | 1/2,1/2,1/2)
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3). \)

Positions

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<thead>
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</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) (x,y,z[u,v,w])</td>
</tr>
<tr>
<td>4 b 2..</td>
<td>(2) (\bar{x},\bar{y},z[u,v,w])</td>
</tr>
<tr>
<td>2 a 4'..</td>
<td>(3) (y,x,z[v,u,w])</td>
</tr>
<tr>
<td></td>
<td>(4) (y,\bar{x},z[v,u,\bar{w}])</td>
</tr>
<tr>
<td></td>
<td>(0,0,0) + (1/2,1/2,1/2) ' +</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p 4
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 1/2,0,z

Along [1,0,0] c1m'1
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p1m'1
\[ a^* = -(a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
Origin on 2
Asymmetric unit \(0 < x < \frac{1}{2}; \quad 0 < y < 1; \quad 0 < z < \frac{1}{4}\)

Symmetry Operations

For \((0,0,0) + \text{ set}\)

(1) 1

(2) \begin{align*}
  2 & 0,0,z \\
  2 & 0,0,0
\end{align*}

(3) \begin{align*}
  4^+ & (0,0,1/4) -1/4,1/4,z \\
  4 & 0,1/2,1/4
\end{align*}

(4) \begin{align*}
  4 & (0,0,1/4) 1/4,1/4,z \\
  4^{-1} & 0,1/2,1/4
\end{align*}

For \((1/2,1/2,1/2) + \text{ set}\)

(1) \begin{align*}
  t & (1/2,1/2,1/2) \\
  t & 1/2,1/2,1/2
\end{align*}

(2) \begin{align*}
  2 & (0,0,1/2) 1/4,1/4,z \\
  2 & 1/2,1/2,1/2
\end{align*}

(3) \begin{align*}
  4^+ & (0,0,3/4) 1/4,1/4,z \\
  4 & 1/2,0,3/4
\end{align*}

(4) \begin{align*}
  4 & (0,0,3/4) 1/4,-1/4,z \\
  4^{-1} & 1/2,0,3/4
\end{align*}
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
</tbody>
</table>

8 b 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x+1/2,z+1/4 [v,u,w] (4) y,x+1/2,z+1/4 [v,u,w]

4 a 2.. 0,0,z [0,0,w] 0,1/2,z+1/4 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p4 Along [1,0,0] c1m'1 Along [1,1,0] p1m'1

\(a^* = (a - b)/2\) \(b^* = (a + b)/2\)

Origin at 1/4,1/4,z Origin at x,0,0 Origin at x,x,0
I4₁₁'
80.2.689
Tetragonal

Origin on 21'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1 
(2) 2 0,0,z 
(3) 4⁺ (0,0,1/4) -1/4,1/4,z 
(4) 4⁻ (0,0,1/4) 1/4,1/4,z

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) 
(2) 2 (0,0,1/2) 1/4,1/4,z 
(3) 4⁺ (0,0,3/4) 1/4,1/4,z 
(4) 4⁻ (0,0,3/4) 1/4,-1/4,z

For (0,0,0)' + set

(1) 1' 
(2) 2' 0,0,z 
(3) 4⁺ ' (0,0,1/4) -1/4,1/4,z 
(4) 4⁻ ' (0,0,1/4) 1/4,1/4,z

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) 
(2) 2' (0,0,1/2) 1/4,1/4,z 
(3) 4⁺ ' (0,0,3/4) 1/4,1/4,z 
(4) 4⁻ ' (0,0,3/4) 1/4,-1/4,z
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
<td>(1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) y,x+1/2,z+1/4 [0,0,0] (4) y,x+1/2,z+1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'  
a* = (a - b)/2  
Origin at 1/4,1/4,z

Along [1,0,0] c1m11'  
a* = b  
b* = c  
Origin at x,0,0

Along [1,1,0] p1m11'  
a* = (a + b)/2  
b* = c/2  
Origin at x,x,0
Origin on 2

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0)$ + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(1) 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(2) 0,0,z</td>
</tr>
<tr>
<td></td>
<td>(3) $4^+ \cdot (0,0,1/4)$, $-1/4,1/4,z$</td>
</tr>
<tr>
<td></td>
<td>(4) $4^- \cdot (0,0,1/4)$, $1/4,1/4,z$</td>
</tr>
</tbody>
</table>

For $(1/2,1/2,1/2) + set$

<table>
<thead>
<tr>
<th>Operation</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $t$</td>
<td>(1) 1/2,1/2,1/2</td>
</tr>
<tr>
<td></td>
<td>(2) $0,0,1/2$</td>
</tr>
<tr>
<td></td>
<td>(3) $4^+ \cdot (0,0,3/4)$, $1/4,1/4,z$</td>
</tr>
<tr>
<td></td>
<td>(4) $4^- \cdot (0,0,3/4)$, $1/4,-1/4,z$</td>
</tr>
</tbody>
</table>

80.3.690 - 1 - 1372
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 a 2</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
</tr>
<tr>
<td>Origin at 1/4,1/4,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2'

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

For \((0,0,0) + \) set

1. \( (1,0,0,0) \)
2. \( 2', 0,0,z \) 
   \( (2_z,0,0) \)
3. \( 4^+ (0,0,1/4) -1/4,1/4,z \) 
   \( (4_z,0,1/2,1/4) \)
4. \( 4^- (0,0,1/4) 1/4,1/4,z \) 
   \( (4_z^{-1},0,1/2,1/4) \)

For \((1/2,1/2,1/2)' + \) set

1. \( t' (1/2,1/2,1/2) \)
   \( (1,1/2,1/2) \)
2. \( 2 (0,0,1/2) 1/4,1/4,z \) 
   \( (2_z,1/2,1/2,1/2) \)
3. \( 4^+ (0,0,3/4) 1/4,1/4,z \) 
   \( (4_z,1/2,0,3/4) \)
4. \( 4^- (0,0,3/4) 1/4,-1/4,z \) 
   \( (4_z^{-1},1/2,0,3/4) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[ (0,0,0) + (1/2,1/2,1/2)' + \]

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x+1/2,z+1/4 [v,u,w] (4) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>4 a'</td>
<td>0,0,z [u,v,0] 0,1/2,z+1/4 [v,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( \mathbf{p}_{\mathbf{c}'} \) 4  
\( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \) Origin at -1/4,1/4,z

Along [1,0,0] \( \mathbf{c}_{\mathbf{p}'} \) \( \mathbf{1m}' \) 1
\( a^* = b \) \( b^* = c \) Origin at x,0,0

Along [1,1,0] \( \mathbf{p}_{2\mathbf{c}} \) \( \mathbf{1m} \) 1
\( a^* = (-a + b)/2 \) \( b^* = c/2 \) Origin at x,x,0
Origin on 2'

Asymmetric unit  
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4\]

Symmetry Operations

For \((0,0,0)\) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2' \quad 0,0,z \\
(3) & \quad 4^{+} \quad (0,0,1/4) -1/4,1/4,z \\
(4) & \quad 4^{-} \quad (0,0,1/4) \quad 1/4,1/4,z \\
\end{align*}
\]

For \((1/2,1/2,1/2)'\) set

\[
\begin{align*}
(1) & \quad t' \quad (1/2,1/2,1/2) \\
(2) & \quad 2 \quad (0,0,1/2) \quad 1/4,1/4,z \\
(3) & \quad 4^{+} \quad (0,0,3/4) \quad 1/4,1/4,z \\
(4) & \quad 4^{-} \quad (0,0,3/4) \quad 1/4,-1/4,z \\
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

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<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x' - y,z [u,v,w]</td>
</tr>
<tr>
<td>4 a 2'..</td>
<td>0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/4 [v,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

| Along          | | Along          | | Along          |
|----------------|-----------------------|-----------------------|-----------------------|
| [0,0,1]  p_4   | a* = (a - b)/2       | [1,0,0] c_{1m1}     | a* = b            |
|              | b* = (a + b)/2       |                      | b* = c            |
| Origin at -1/4,1/4,z | Origin at x,0,0   | Origin at x,x,0     |
Origin on \( \bar{4} \)

Asymmetric unit: \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1 \)

Symmetry Operations:

1. \((1)\ 1 \)
   \((1|0,0,0)\)

2. \((2)\ 2\ 0,0,z \)
   \((2|0,0,0)\)

3. \((3)\ \bar{4}\ 0,0,z;\ 0,0,0 \)
   \((4|0,0,0)\)

4. \((4)\ \bar{4}\ 0,0,z;\ 0,0,0 \)
   \((4|0,0,0)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3).

Positions

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<td>4 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>2 g 2..</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 f 2..</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 e 2..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1 d 4..</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 c 4..</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>1 b 4..</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 a 4..</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'  
\( a^* = a \)  \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p1m'1  
\( a^* = b \)  \( b^* = c \)  
Origin at x,0,0

Along [1,1,0] p1m'1  
\( a^* = (-a + b)/2 \)  \( b^* = c \)  
Origin at x,x,0
Origin on $\overline{4}1'$

Asymmetric unit $\quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For $1 + set$

(1) $1$ \hspace{1cm} (2) $2 \cdot 0,0,z$ \hspace{1cm} (3) $\overline{4}$ $\cdot 0,0,z;\ 0,0,0$ \hspace{1cm} (4) $\overline{4}$ $\cdot 0,0,z;\ 0,0,0$

$\quad (1) 0,0,0$ \hspace{1cm} $\quad (2_z|0,0,0)$ \hspace{1cm} $\quad (4_z|0,0,0)$ \hspace{1cm} $\quad (4_z'|0,0,0)$

For $1' + set$

(1) $1'$ \hspace{1cm} (2) $2' \cdot 0,0,z'\hspace{1cm} (3) \overline{4}' \cdot 0,0,z';\ 0,0,0$ \hspace{1cm} (4) $\overline{4}' \cdot 0,0,z';\ 0,0,0$

$\quad (1) 0,0,0'$ \hspace{1cm} $\quad (2_z|0,0,0)'$ \hspace{1cm} $\quad (4_z|0,0,0)'$ \hspace{1cm} $\quad (4_z'|0,0,0)'$
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>1 + 1'</td>
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</tr>
<tr>
<td>4 h 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>2 g 2..1'</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 f 2..1'</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 e 2..1'</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>1 d 4..1'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 c 4..1'</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b 4..1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a 4..1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**  p41'
  - \( a^* = a \)
  - \( b^* = b \)
  - Origin at 0,0,z

- **Along [1,0,0]**  p1m1'
  - \( a^* = b \)
  - \( b^* = c \)
  - Origin at x,0,0

- **Along [1,1,0]**  p1m1'
  - \( a^* = (-a + b)/2 \)
  - \( b^* = c \)
  - Origin at x,x,0
Origin on \( \alpha' \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1 \)

Symmetry Operations

(1) 1
(1*0,0,0)

(2) \( z \quad 0,0,z \)
(2*0,0,0)

(3) \( \alpha' \quad 0,0,z; \quad 0,0,0 \)
(\( \alpha_2 \quad 0,0,0' \))

(4) \( \alpha' \quad 0,0,z; \quad 0,0,0 \)
(\( \alpha_2^{-1*0,0,0} \))

Tetragonal

81.3.695 P\&'

P\&'

81.3.695
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
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<td>( (1) \ x, y, z \ [u, v, w] )</td>
</tr>
<tr>
<td>( 2 ) g 2..</td>
<td>( 0,1/2,z \ [0,0,w] )</td>
</tr>
<tr>
<td>( 2 ) f 2..</td>
<td>( 1/2,1/2,z \ [0,0,w] )</td>
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<tr>
<td>( 2 ) e 2..</td>
<td>( 0,0,z \ [0,0,w] )</td>
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<tr>
<td>( 1 ) d</td>
<td>( 1/2,1/2,1/2 \ [0,0,0] )</td>
</tr>
<tr>
<td>( 1 ) c</td>
<td>( 1/2,1/2,0 \ [0,0,0] )</td>
</tr>
<tr>
<td>( 1 ) b</td>
<td>( 0,0,1/2 \ [0,0,0] )</td>
</tr>
<tr>
<td>( 1 ) a</td>
<td>( 0,0,0 \ [0,0,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \( p4 \)
  - \( a^* = a \) \( b^* = b \)
  - Origin at 0,0,z

- Along \([1,0,0]\) \( p1m'1 \)
  - \( a^* = b \) \( b^* = c \)
  - Origin at x,0,0

- Along \([1,1,0]\) \( p1m'1 \)
  - \( a^* = (-a + b)/2 \) \( b^* = c \)
  - Origin at x,x,0
P2c 4
81.4.696

41'
81.4.696
P2c 4

Origin on $\overline{4}$

Asymmetric unit

$x: 0 \leq x \leq 1/2; \quad y: 0 \leq y \leq 1/2; \quad z: 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

$\begin{align*}
(1) & \quad 1 \\
(1 \mid 0,0,0) & \quad (2) \quad 2 \quad 0,0,z \\
(2_z \mid 0,0,0) & \quad (3) \quad 4^* \quad 0,0,z; \quad 0,0,0 \\
(4 \mid 0,0,0) & \quad (4_z \mid 0,0,0)
\end{align*}$

For (0,0,1)$'$ + set

$\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(1 \mid 0,0,1)' & \quad (2) \quad 2' \quad (0,0,1) \quad 0,0,z \\
(2_z \mid 0,0,1)' & \quad (3) \quad 4^* \quad 0,0,z; \quad 0,0,1/2 \\
(4 \mid 0,0,1)' & \quad (4_z \mid 0,0,1)'
\end{align*}$
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3).

**Positions**

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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>8</td>
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<td>(0,0,0) +</td>
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<td>4</td>
<td>g 2.. 0,1/2,z [0,0,w]</td>
<td>(0,0,1) +</td>
</tr>
<tr>
<td>4</td>
<td>f 2.. 1/2,1/2,z [0,0,w]</td>
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</tr>
<tr>
<td>4</td>
<td>e 2.. 0,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>d 4.. 1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>c 4.. 1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b 4.. 0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a 4.. 0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  p41'  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0]  p_{2b'}m1'  
\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,0,0

Along [1,1,0]  p_{2b'}m1'  
\[ \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,0
Origin on $4$

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

**Symmetry Operations**

For \((0,0,0) + \) set

\[(1) \quad 1 \quad (2) \quad 2 \quad (3) \quad 4^+ \quad (4) \quad 4^-\]

\[(1) \quad (0,0,0) \quad (2) \quad (0,0,z) \quad (3) \quad (0,0,0) \quad (4) \quad (0,0,0)\]

\[(1) \quad (1,0,0) \quad (2) \quad (2z,0,0) \quad (3) \quad (4z,0,0) \quad (4) \quad (4z^1,0,0)\]

For \((1,0,0) + \) set

\[(1) \quad t'(1,0,0) \quad (2) \quad 2' \quad 1/2,0,z \quad (3) \quad 4'^- \quad 1/2,1/2,z; \quad 1/2,1/2,0 \quad (4) \quad 4'^- \quad 1/2,1/2,0; \quad 1/2,1/2,0\]

\[(1) \quad (1,0,0)' \quad (2) \quad (2z,1,0,0)' \quad (3) \quad (4z,1,0,0)' \quad (4) \quad (4z^1,1,0,0)'\]
Generators selected  (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3).

Positions

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<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>8 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 g 2'..</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 f 2'..</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 2'..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d 4'..</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 4'..</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b 4'..</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 4'..</td>
<td>0,0,0 [0,0,w]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p\text{p}_{\text{c}} 4</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [1,1,0] p_{\text{2c}}1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = a  b^* = b</td>
<td>a^* = b  b^* = c</td>
<td>a^* = (-a + b)/2  b^* = c</td>
</tr>
<tr>
<td>Origin at 1/2,1/2,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x-1/4,x+1/4,0</td>
</tr>
</tbody>
</table>
Origin on $\overline{4}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

(0,0,0) + set

1

$1 | 0,0,0$

2 $0,0,z$

$2 | 0,0,0$

$\overline{4}$ $0,0,0$

$\overline{4} | 0,0,0$

$\overline{4}$ $0,0,0$

$\overline{4} | 0,0,0$

For $(1,0,0)' + set$

$1'$ $(1,0,0)$

$1' | 1,0,0$

$2' 1/2,0,z$

$2' | 1,0,0$

$\overline{4}' 1/2,1/2,0$

$\overline{4}' | 1,0,0$

$\overline{4}' 1/2,1/2,0$

$\overline{4}' | 1,0,0$
Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3).

Positions

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>8 h 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 g 2'..</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 f 2..</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 2..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d 4'..</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c 4'..</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b 4'..</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 4'..</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'  
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p1m11'  
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p_{c1}m1  
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x-1/4,x+1/4,0
Origin on \(\overline{4}\)

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1\)

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \(1\) \(0,0,0\)
2. \(2\) \(0,0,z\)
3. \(4\) \(0,0,0\)
4. \(4\) \(0,0,0\)

For \((1/2,1/2,1/2) + \text{set}\)

1. \(t\) \(1/2,1/2,1/2\)
2. \(2\) \(0,0,1/2\)
3. \(4\) \(1/2,0,z\)
4. \(4\) \(0,1/2,z\)

\(82.1.699 - 1\ - 1390\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>4 f 2..</td>
<td>0,1/2,z [0,0,w]</td>
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<tr>
<td>4 e 2..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d 4..</td>
<td>0,1/2,3/4 [0,0,w]</td>
</tr>
<tr>
<td>2 c 4..</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td>2 b 4..</td>
<td>0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0,0 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'  
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] c1m'1  
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p1m'1  
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
Origin on $\overline{4}1'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1$

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2 | 0,0,0)

(3) $\overline{4}$' 0,0,0; 0,0,0
($4_z | 0,0,0$)

(4) $\overline{4}$' 0,0,z; 0,0,0
($4_z^{-1} | 0,0,0$)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2 | 1/2,1/2,1/2)

(3) $\overline{4}$' 1/2,0,z; 1/2,0,1/4
($4_z | 1/2,1/2,1/2$)

(4) $\overline{4}$' 0,1/2,z; 0,1/2,1/4
($4_z^{-1} | 1/2,1/2,1/2$)

For (0,0,0)'+ set

(1) 1'
(1 | 0,0,0)

(2) 2' 0,0,z
(2 | 0,0,0)

(3) $\overline{4}$' 0,0,0; 0,0,0
($4_z | 0,0,0$)

(4) $\overline{4}$' 0,0,z; 0,0,0
($4_z^{-1} | 0,0,0$)

For (1/2,1/2,1/2)'+ set

(1) t' (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)

(2) 2' (0,0,1/2) 1/4,1/4,z
(2 | 1/2,1/2,1/2)

(3) $\overline{4}$' 1/2,0,z; 1/2,0,1/4
($4_z | 1/2,1/2,1/2$)

(4) $\overline{4}$' 0,1/2,z; 0,1/2,1/4
($4_z^{-1} | 1/2,1/2,1/2$)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3);1'.

Positions

<table>
<thead>
<tr>
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<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 11'</td>
<td>(1) x,y,z</td>
<td>(2) x,y,z</td>
<td>(3) y,x,z</td>
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<td>4 f 2..1'</td>
<td>0,1/2,z</td>
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<td>1/2,0,z</td>
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<tr>
<td>4 e 2..1'</td>
<td>0,0,z</td>
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<td>0,0,z</td>
</tr>
<tr>
<td>2 d 4..1'</td>
<td>0,1/2,3/4</td>
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<tr>
<td>2 c 4..1'</td>
<td>0,1/2,1/4</td>
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</tr>
<tr>
<td>2 b 4..1'</td>
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<tr>
<td>2 a 4..1'</td>
<td>0,0,0</td>
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</table>

Symmetry of Special Projections

Along [0,0,1]  p41'  Along [1,0,0]  c1m11'  Along [1,1,0]  p1m11'
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z  \[ a^* = b \quad b^* = c \]
Origin at x,0,0  \[ a^* = (a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
82.3.701

Tetragonal

I4'  

82.3.701  I4'

Asymmetric unit

0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 0,0,0)

(2) 2  0,0,z
(2z 0,0,0)

(3) 4^-  0,0,z; 0,0,0
(4z 0,0,0')

(4) 4^-  0,0,z; 0,0,0
(4z^{-1} 0,0,0')

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2z 1/2,1/2,1/2)

(3) 4^-  1/2,0,z; 1/2,0,1/4
(4z 1/2,1/2,1/2')

(4) 4^-  1/2,0,z; 1/2,0,1/4
(4z^{-1} 1/2,1/2,1/2')
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3).

<table>
<thead>
<tr>
<th>Positions</th>
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<tbody>
<tr>
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<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 f 2..</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 2..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d 4'..</td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 c 4'..</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2 b 4'..</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 4'..</td>
<td>0,0,0 [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4</th>
<th>Along [1,0,0]</th>
<th>c1m'1</th>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
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<tbody>
<tr>
<td>a' = (a - b)/2</td>
<td>b' = (a + b)/2</td>
<td>a' = b</td>
<td>b' = c</td>
<td>a' = (-a + b)/2</td>
<td>b' = c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0
Origin on $\bar{4}$

Asymmetric unit 0 ≤ $x$ ≤ 1/2; 0 ≤ $y$ ≤ 1/2; 0 ≤ $z$ ≤ 1

Symmetry Operations

For (0,0,0) + set

1. $\bar{1}$
   
2. $\bar{2}$, 0,0,z
   
3. $\bar{4}^+$, 0,0,z; 0,0,0
   
4. $\bar{4}^-$, 0,0,z; 0,0,0

For $(1/2,1/2,1/2)' + set$

1. $t'(1/2,1/2,1/2)$
2. $2'(0,0,1/2)$, 1/4,1/4,z
3. $\bar{4}^{+*}$, 1/2,0,z; 1/2,0,1/4
4. $\bar{4}^{-*}$, 0,1/2,z; 0,1/2,1/4

82.4.702 - 1 - 1396
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1)</td>
<td></td>
</tr>
<tr>
<td>4 f 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 e 2..</td>
<td>0,0,z [0,0,w]</td>
<td>(3) x,y,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>2 d 4'..</td>
<td>0,1/2,3/4 [0,0,0]</td>
<td>(4) x,y,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>2 c 4'..</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>(3) x,y,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 4'..</td>
<td>0,0,1/2 [0,0,0]</td>
<td>(4) x,y,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>2 a 4'..</td>
<td>0,0,0 [0,0,0]</td>
<td>(4) x,y,z [v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1]  $p_4$ 4
  - $a^* = (a - b)/2$  $b^* = (a + b)/2$
  - Origin at 1/2,0,z

- Along [1,0,0]  $c_{1m1}$
  - $a^* = b$  $b^* = c$
  - Origin at x,0,0

- Along [1,1,0]  $p_{21m1}$
  - $a^* = (a + b)/2$  $b^* = c/2$
  - Origin at x,x,0
Origin at center (4/m)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. \(1\)
   \[ (1 | 0,0,0) \]

2. \(2\)
   \[ 0,0,z \]
   \[ (2_z | 0,0,0) \]

3. \(4^+\)
   \[ 0,0,z \]
   \[ (4_z | 0,0,0) \]

4. \(4^-\)
   \[ 0,0,z \]
   \[ (4_z^{-1} | 0,0,0) \]

5. \(\overline{1}\)
   \[ 0,0,0 \]
   \[ (1 | 0,0,0) \]

6. \(m\)
   \[ x,y,0 \]
   \[ (m_z | 0,0,0) \]

7. \(\overline{4}^+\)
   \[ 0,0,z; 0,0,0 \]
   \[ (4_z | 0,0,0) \]

8. \(\overline{4}^-\)
   \[ 0,0,z; 0,0,0 \]
   \[ (4_z^{-1} | 0,0,0) \]
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>(1) x,y,z [u,v,w] (2) (x, y, z \ [u, v, w]) (3) (y, x, z \ [v, u, w]) (4) (y, x, z \ [v, u, w]) (5) (x, y, z \ [u, v, w]) (6) (x, y, z \ [u, v, w]) (7) (y, x, z \ [v, u, w]) (8) (y, x, z \ [v, u, w])</td>
</tr>
<tr>
<td>4 k m..</td>
<td>x,y,1/2 [0,0,w] (x, y, 1/2 \ [0,0,w]) (y, x, 1/2 \ [0,0,w]) y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 j m..</td>
<td>x,y,0 [0,0,w] (x, y, 0 \ [0,0,w]) (y, x, 0 \ [0,0,w]) y,x,0 [0,0,w]</td>
</tr>
<tr>
<td>4 l 2..</td>
<td>0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 0,1/2,z [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 h 4..</td>
<td>1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 g 4..</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 f 2/m..</td>
<td>0,1/2,1/2 [0,0,w] 1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 e 2/m..</td>
<td>0,1/2,0 [0,0,w] 1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>1 d 4/m..</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 c 4/m..</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>1 b 4/m..</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 a 4/m..</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]** p41’  
  \(a^* = a \quad b^* = b\)  
  Origin at 0,0,z

- **Along [1,0,0]** p2’mm’  
  \(a^* = -c \quad b^* = b\)  
  Origin at x,0,0

- **Along [1,1,0]** p2’mm’  
  \(a^* = -c \quad b^* = (-a + b)/2\)  
  Origin at x,x,0
Origin at center (4/m1')

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For 1 + set

(1) 1  
(1|0,0,0)

(2) 2  0,0,z  
(2_z|0,0,0)

(3) 4* 0,0,z  
(4_z|0,0,0)

(4) 4* 0,0,z  
(4_z^{-1}|0,0,0)

(5) \(\bar{1}\) 0,0,0  
(1|0,0,0)

(6) m x,y,0  
(m_z|0,0,0)

(7) \(\bar{4}\)* 0,0,z; 0,0,0  
(4_z|0,0,0)

(8) \(\bar{4}\)* 0,0,z; 0,0,0  
(4_z^{-1}|0,0,0)

For 1' + set

(1) 1'  
(1|0,0,0)'

(2) 2'  0,0,z  
(2_z|0,0,0)'

(3) 4'* 0,0,z  
(4_z|0,0,0)'

(4) 4'* 0,0,z  
(4_z^{-1}|0,0,0)'

(5) \(\bar{1}\)' 0,0,0  
(1|0,0,0)'

(6) m' x,y,0  
(m_z|0,0,0)'

(7) \(\bar{4}\)'* 0,0,z;0,0,0  
(4_z|0,0,0)'

(8) \(\bar{4}\)'* 0,0,z;0,0,0  
(4_z^{-1}|0,0,0)'

83.2.704 - 1 - 1400
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>11'</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y, x, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) y, x, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(6) x, y, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) y, x, z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(8) y, x, z [0,0,0]</td>
</tr>
</tbody>
</table>

| 4            | m..1'       |
|              | x,y,1/2 [0,0,0] |
|              | x,y,1/2 [0,0,0] |
|              | y,x,1/2 [0,0,0] |
|              | y,x,1/2 [0,0,0] |

| 4            | m..1'       |
|              | x,y,0 [0,0,0] |
|              | x,y,0 [0,0,0] |
|              | y,x,0 [0,0,0] |
|              | y,x,0 [0,0,0] |

| 4            | l 2..1'     |
|              | 0,1/2,z [0,0,0] |
|              | 1/2,0,z [0,0,0] |
|              | 0,1/2,z [0,0,0] |
|              | 1/2,0,z [0,0,0] |

| 2            | h 4..1'     |
|              | 1/2,1/2,z [0,0,0] |
|              | 1/2,1/2,z [0,0,0] |

| 2            | g 4..1'     |
|              | 0,0,z [0,0,0] |
|              | 0,0,z [0,0,0] |

| 2            | f 2/m..1'   |
|              | 0,1/2,1/2 [0,0,0] |
|              | 1/2,0,1/2 [0,0,0] |

| 2            | e 2/m..1'   |
|              | 0,1/2,0 [0,0,0] |
|              | 1/2,0,0 [0,0,0] |

| 1            | d 4/m..1'   |
|              | 1/2,1/2,1/2 [0,0,0] |

| 1            | c 4/m..1'   |
|              | 1/2,1/2,0 [0,0,0] |

| 1            | b 4/m..1'   |
|              | 0,0,1/2 [0,0,0] |

| 1            | a 4/m..1'   |
|              | 0,0,0 [0,0,0] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p41'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (4'/m)

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

1. \(1\)
   \[(1|0,0,0)\]

2. \(2\)
   \[
   \begin{cases} 
   0,0,z \\
   (2_z|0,0,0)
   \end{cases}
   \]

3. \(4^+\cdot\)
   \[
   \begin{cases} 
   0,0,z \\
   (4_z|0,0,0')
   \end{cases}
   \]

4. \(4^-\cdot\)
   \[
   \begin{cases} 
   0,0,z \\
   (4_z^{-1}|0,0,0')
   \end{cases}
   \]

5. \(1\)
   \[(1|0,0,0)\]

6. \(m\)
   \[
   \begin{cases} 
   x,y,0 \\
   (m_z|0,0,0)
   \end{cases}
   \]

7. \(4^{+}\cdot\)
   \[
   \begin{cases} 
   0,0,z; 0,0,0 \\
   (4_z|0,0,0')
   \end{cases}
   \]

8. \(4^{-}\cdot\)
   \[
   \begin{cases} 
   0,0,z; 0,0,0 \\
   (4_z^{-1}|0,0,0')
   \end{cases}
   \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>x,y,z [u,v,w]</td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>5 x, y, z [u, v, w]</td>
<td>(6) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>4 k m..</td>
<td>x,y,1/2 [0,0,w]</td>
<td>x, y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 j m..</td>
<td>x,y,0 [0,0,w]</td>
<td>x, y,0 [0,0,w]</td>
</tr>
<tr>
<td>4 l 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 h 4'..</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 g 4'..</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 f 2/m..</td>
<td>0,1/2,1/2 [0,0,w]</td>
<td>1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 e 2/m..</td>
<td>0,1/2,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>1 d 4'/m..</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 c 4'/m..</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 b 4'/m..</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a 4'/m..</td>
<td>0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>p41'</th>
<th>p2' mm'</th>
<th>p2' mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>a* = a</td>
<td>a* = -c</td>
<td>a* = -c</td>
</tr>
<tr>
<td></td>
<td>b* = b</td>
<td>b* = b</td>
<td>b* = (-a + b)/2</td>
</tr>
<tr>
<td></td>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin at center (4/m’)

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations:

1. \(1\) 0,0,0
2. \(2\) 0,0,\(z\) (2\(z\)) 0,0,0
3. \(4\) 0,0,\(z\) (4\(z\)) 0,0,0
4. \(4\) 0,0,\(z\) (4\(z\)) -1 0,0,0
5. \(\overline{1}\) 0,0,0 (1,0,0,0)
6. \(m\) 0,0,0 (0,0,0)
7. \(\overline{4}\) 0,0,\(z\) (0,0,0) (4\(z\)) 0,0,0
8. \(\overline{4}\) 0,0,\(z\) (0,0,0) (4\(z\)) -1 0,0,0

83.4.706 - 1 - 1404
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 k</td>
<td>2</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 j</td>
<td>2</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>4 l 2..</td>
<td>2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 h</td>
<td>4</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 g</td>
<td>4</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 f</td>
<td>2/m'..</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 e</td>
<td>2/m'..</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1 d</td>
<td>4/m'..</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 c</td>
<td>4/m'..</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b</td>
<td>4/m'..</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a</td>
<td>4/m'..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p41'  Along [1,0,0]  p2m'm'  Along [1,1,0]  p2m'm'

a* = a  b* = b  a* = b  b* = c  a* = (-a + b)/2  b* = c

Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
Origin at center (4'/m'')

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

1. \(1\) \((0,0,0)\)
2. \(2\) \(0,0,z\) \((2z,0,0)\)
3. \(4^+\) \(0,0,z\) \((4z,0,0,0)'\)
4. \(4^-\) \(0,0,z\) \((4z^{-1},0,0,0)'\)
5. \(T\) \(0,0,0\) \((1,0,0,0)'\)
6. \(m'\) \(x,y,0\) \((m_z,0,0,0)'\)
7. \(4^+\) \(0,0,z\) \((4z,0,0,0)'\)
8. \(4^-\) \(0,0,z\) \((4z^{-1},0,0,0)'\)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 k m'..</td>
<td>x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 j m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>4 l 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 h 4'..</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 g 4'..</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 f 2/m'..</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 e 2/m'..</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>1 d 4'/m'..</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 c 4'/m'..</td>
<td>1/2,1/2,0 [0,0,0]</td>
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</tr>
<tr>
<td>1 b 4'/m'..</td>
<td>0,0,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>1 a 4'/m'..</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'</th>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td></td>
<td>b* = b</td>
<td></td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at center (4/m)

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

**For (0,0,0) + set**

(1) 1

(2) 2 0,0,z

(3) 4+ 0,0,z

(4) 4− 0,0,z

For (0,0,1)' + set

(5) $t'$ (0,0,1)

(6) m x,y,0

(7) 4+ (0,0,1) 0,0,z

(8) 4− (0,0,1) 0,0,z

(1) 1 (0,0,0)

(2) 2 0,0,z

(3) 4+ 0,0,z

(4) 4− 0,0,z

(5) $t'$ (0,0,1)

(6) m x,y,0

(7) 4+ (0,0,1) 0,0,z

(8) 4− (0,0,1) 0,0,z

(1) t (0,0,1)

(2) 2 (0,0,1) 0,0,z

(3) 4+ (0,0,1) 0,0,z

(4) 4− (0,0,1) 0,0,z

(5) $t'$ (0,0,1/2)

(6) m' x,y,1/2

(7) 4+ (0,0,1/2) 0,z

(8) 4− (0,0,1/2) 0,z

(1) t (0,0,1)

(2) 2 (0,0,1) 0,0,z

(3) 4+ (0,0,1) 0,0,z

(4) 4− (0,0,1) 0,0,z

(5) $t'$ (0,0,1/2)

(6) m' x,y,1/2

(7) 4+ (0,0,1/2) 0,z

(8) 4− (0,0,1/2) 0,z
Generators selected  

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 I 1</td>
<td>x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z</td>
<td>(0,0,1)' +</td>
</tr>
<tr>
<td>8 k m'..</td>
<td>x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 j m..</td>
<td>x,y,0 [0,0,w]</td>
<td>y,x,0 [0,0,w]</td>
</tr>
<tr>
<td>8 l 2..</td>
<td>0,1/2, z [0,0,w]</td>
<td>1/2,0, z [0,0,w]</td>
</tr>
<tr>
<td>4 h 4..</td>
<td>1/2, 1/2, z [0,0,w]</td>
<td>1/2,1/2, z [0,0,w]</td>
</tr>
<tr>
<td>4 g 4..</td>
<td>0, 0, z [0,0,w]</td>
<td>0,0, z [0,0,w]</td>
</tr>
<tr>
<td>4 f 2/m'..</td>
<td>0, 1/2, 1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e 2/m..</td>
<td>0, 1/2, 0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2 d 4/m'..</td>
<td>1/2, 1/2, 1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 c 4/m..</td>
<td>1/2, 1/2, 0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 4/m'..</td>
<td>0, 0, 1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 4/m..</td>
<td>0, 0, 0 [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**  
  \( p41' \)  
  \( \mathbf{a}^* = \mathbf{a} \)  
  \( \mathbf{b}^* = \mathbf{b} \)  
  \( \mathbf{c}^* = \mathbf{c} \)  
  Origin at 0,0, z

- **Along [1,0,0]**  
  \( p_{2a}{2m'} \)  
  \( \mathbf{a}^* = -\mathbf{c} \)  
  \( \mathbf{b}^* = \mathbf{b} \)  
  \( \mathbf{c}^* = \mathbf{c} \)  
  Origin at x,0,1/2

- **Along [1,1,0]**  
  \( p_{2a}{2m'} \)  
  \( \mathbf{a}^* = -\mathbf{c} \)  
  \( \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)  
  \( \mathbf{c}^* = \mathbf{c} \)  
  Origin at x,x,1/2
**Origin** at center \((4/m)\)

**Asymmetric unit**  
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \((1,0,0,0)\)
2. \((0,0,z)\)  
   \((m,0,0,0)\)
3. \((0,0,z)\)  
   \((m,0,0,0)\)
4. \((0,0,z)\)  
   \((m,0,0,0)\)

For \((1,0,0)\) ′ + set

1. \((1,0,0,0)\) ′
2. \((2,1/2,0,0)\) ′
3. \((4,1/2,1/2,0)\) ′
4. \((4,1/2,-1/2,0)\) ′

83.7.709 - 1 - 1410
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
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<td>(0,0,0) +</td>
<td>(1,0,0)′ +</td>
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<table>
<thead>
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</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 k</td>
<td>x,y,1/2 [0,0,w]</td>
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<td>x,y,1/2 [0,0,w]</td>
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<tr>
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<td>y,x,1/2 [0,0,w]</td>
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<td></td>
<td>y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 j</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
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<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>y,x,0 [0,0,w]</td>
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<tr>
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<td>y,x,0 [0,0,w]</td>
</tr>
<tr>
<td>8 l</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
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<td>1/2,0,z [v,u,0]</td>
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<tr>
<td></td>
<td>1/2,0,z [v,u,0]</td>
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<tr>
<td>4 h</td>
<td>1/2,1/2,z [0,0,0]</td>
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<td>1/2,1/2,z [0,0,0]</td>
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<tr>
<td>4 g</td>
<td>0,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 f</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<td>1/2,0,0 [0,0,0]</td>
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<tr>
<td>2 d</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>2 c</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>2 b</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

**Along [0,0,1]**

- \( p41' \)
- \( a^* = a \quad b^* = b \)
- Origin at 0,0,z

**Along [1,0,0]**

- \( p2mm1' \)
- \( a^* = b \quad b^* = c \)
- Origin at x,0,0

**Along [1,1,0]**

- \( p2m'm' \)
- \( a^* = (-a + b)/2 \quad b^* = c \)
- Origin at x-1/4,x+1/4,0
Origin at center (4/m)

Asymmetric unit \(0 \leq x \leq 1/2;\quad 0 \leq y \leq 1/2;\quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0)\) + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>((1</td>
</tr>
<tr>
<td>2</td>
<td>((0,0,z)) ((2z</td>
</tr>
<tr>
<td>3</td>
<td>((4^+ 0,0,z)) ((4z</td>
</tr>
<tr>
<td>4</td>
<td>((4^- 0,0,z)) ((4z^{-1}</td>
</tr>
<tr>
<td>5</td>
<td>((0,0,0)) ((1</td>
</tr>
<tr>
<td>6</td>
<td>((x,y,0)) ((mz</td>
</tr>
<tr>
<td>7</td>
<td>((4^+ 0,0,z)) ((4z</td>
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<td>8</td>
<td>((4^- 0,0,z)) ((4z^{-1}</td>
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For \((1,0,0)\)' + set

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<tr>
<td>1</td>
<td>((1</td>
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<tr>
<td>2</td>
<td>((1/2,0,0)) ((2z</td>
</tr>
<tr>
<td>3</td>
<td>((4^+ 1/2,1/2,z)) ((4z</td>
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<tr>
<td>4</td>
<td>((4^- 1/2,-1/2,z)) ((4z^{-1}</td>
</tr>
<tr>
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<td>8</td>
<td>((4^- 1/2,1/2,z)) ((4z^{-1}</td>
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Continued

Generators selected  (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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<tr>
<td>8 k m'</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 j m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 l 2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 h 4'</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 g 4..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 f 2'/m'</td>
<td>0,1/2,1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 e 2'/m</td>
<td>0,1/2,0 [0,0,0]</td>
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<tr>
<td>2 d 4'/m'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2 c 4'/m</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>2 b 4'/m</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 4/m</td>
<td>0,0,0 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

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<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p41'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b b* = c</td>
<td></td>
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<tr>
<td>Origin at x,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
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<th>p,, 2mm</th>
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<tbody>
<tr>
<td>a* = (-a + b)/2 b* = c</td>
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<tr>
<td>Origin at x-1/4,x+1/4,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (4'/m)

Asymmetric unit  

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}\]

Symmetry Operations

For \((0,0,0)\) + set

\[\begin{align*}
(1) & \begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix} \\
(2) & \begin{pmatrix} 2 \\ 0,0,z \end{pmatrix} \quad (2_z | 0,0,0) \\
(3) & \begin{pmatrix} 4^+ \end{pmatrix} \begin{pmatrix} 0,0,z \end{pmatrix} \quad (4_z | 0,0,0) \\
(4) & \begin{pmatrix} 4^- \end{pmatrix} \begin{pmatrix} 0,0,z \end{pmatrix} \quad (4_z^{-1} | 0,0,0) \\
(5) & \begin{pmatrix} T \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} \quad (1 | 0,0,0) \\
(6) & \begin{pmatrix} m \end{pmatrix} \begin{pmatrix} x,y,0 \end{pmatrix} \quad (m_z | 0,0,0) \\
(7) & \begin{pmatrix} 4^+ \end{pmatrix} \begin{pmatrix} 0,0,z; 0,0,0 \end{pmatrix} \quad (4_z | 0,0,0) \\
(8) & \begin{pmatrix} 4^- \end{pmatrix} \begin{pmatrix} 0,0,z; 0,0,0 \end{pmatrix} \quad (4_z^{-1} | 0,0,0) \\
\end{align*}\]

For \((0,0,1)'\) + set

\[\begin{align*}
(1) & \begin{pmatrix} t' \end{pmatrix} \begin{pmatrix} 0,0,1 \end{pmatrix} \quad (1 | 0,0,1) \\
(2) & \begin{pmatrix} 2' \end{pmatrix} \begin{pmatrix} 0,0,1 \end{pmatrix} \quad (2_z | 0,0,1) \\
(3) & \begin{pmatrix} 4^+ \end{pmatrix} \begin{pmatrix} 0,0,1 \end{pmatrix} \quad (4_z | 0,0,1) \\
(4) & \begin{pmatrix} 4^- \end{pmatrix} \begin{pmatrix} 0,0,1 \end{pmatrix} \quad (4_z^{-1} | 0,0,1) \\
(5) & \begin{pmatrix} T' \end{pmatrix} \begin{pmatrix} 0,0,1/2 \end{pmatrix} \quad (1 | 0,0,1) \\
(6) & \begin{pmatrix} m' \end{pmatrix} \begin{pmatrix} x,y,1/2 \end{pmatrix} \quad (m_z | 0,0,1) \\
(7) & \begin{pmatrix} 4^+ \end{pmatrix} \begin{pmatrix} 0,0,z; 0,0,1/2 \end{pmatrix} \quad (4_z | 0,0,1) \\
(8) & \begin{pmatrix} 4^- \end{pmatrix} \begin{pmatrix} 0,0,z; 0,0,1/2 \end{pmatrix} \quad (4_z^{-1} | 0,0,1) \\
\end{align*}\]
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Coordinates
Wyckoff letter, Site Symmetry.

(0,0,0) + (0,0,1)'

16  l  1  (1) x,y,z [u,v,w]  (2) x, y,z [u, v, w]  (3) y, x,z [v, u, w]  (4) y, x,z [v, u, w]
(5) x, y,z [u,v,w]  (6) x,y,z [v,u,w]  (7) y, x,z [v,u,w]  (8) y, x,z [v,u,w]
8  k  2m'..  x,y,1/2 [u,v,0]  x, y,1/2 [u, v, 0]  y, x,1/2 [v, u,0]  y, x,1/2 [v, u,0]
8  j  m..  x,y,0 [0,0,w]  x, y,0 [0,0,w]  y, x,0 [0,0,w]  y, x,0 [0,0,w]
8  l  2..  0,1/2,z [0,0,w]  1/2,0,z [0,0,w]  0,1/2,z [0,0,w]  1/2,0,z [0,0,w]
4  h  4'..  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]
4  g  4'..  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]
4  f  2/m'..  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]
4  e  2/m..  0,1/2,0 [0,0,w]  1/2,0,0 [0,0,w]  1/2,0,0 [0,0,w]  1/2,0,0 [0,0,w]
2  d  4'/m'..  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]
2  c  4'/m..  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]
2  b  4'/m'..  0,0,1/2 [0,0,0]  0,0,1/2 [0,0,0]  0,0,1/2 [0,0,0]  0,0,1/2 [0,0,0]
2  a  4'/m..  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p41'  Along [1,0,0]  p22'  Along [1,1,0]  p22' 2mm'

a* = a  b* = b  a* = -c  b* = b  a* = -c  b* = (-a+b)/2
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
**Origin** at center (4/m' )

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For (0,0,0) + set

1. \( 1 \)
2. \( 2 \) 0,0,z
   \( (2z,0,0) \)
3. \( 4^+ \) 0,0,z
   \( (4z,0,0) \)
4. \( 4^- \) 0,0,z
   \( (4z^{-1},0,0) \)
5. \( \bar{1} \) 0,0,0
   \( (1,0,0) \)
6. m' x,y,0
   \( (mz,0,0) \)
7. \( \bar{4}^{+*} \) 0,0,z; 0,0,0
   \( (4z,0,0) \)
8. \( \bar{4}^{-*} \) 0,0,z; 0,0,0
   \( (4z^{-1},0,0) \)

For (1,0,0)' + set

1. \( t' \)
   \( (1,0,0) \)
2. \( \bar{2} \) 1/2,0,z
   \( (2z,1,0) \)
3. \( \bar{4}^{+*} \) 1/2,1/2,z
   \( (4z,1,0) \)
4. \( \bar{4}^{-*} \) 1/2,-1/2,z
   \( (4z^{-1},1,0) \)
5. \( \bar{1} \) 1/2,0,0
   \( (1,0,0) \)
6. a x,y,0
   \( (mz,1,0) \)
7. \( \bar{4}^{+} \) 1/2,-1/2,z; 1/2,-1/2,0
   \( (4z,1,0) \)
8. \( \bar{4}^{-} \) 1/2,1/2,z; 1/2,1/2,0
   \( (4z^{-1},1,0) \)
**Generators selected**  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(1,0,0)' +</th>
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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
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<tr>
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<td>(6) x,y,z [u,v,w]</td>
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</tr>
<tr>
<td>8 k m..</td>
<td>x,y,1/2 [0,0,w]</td>
<td>x,y,1/2 [0,0,w]</td>
<td>y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 j m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
<td>y,x,0 [v,u,0]</td>
</tr>
<tr>
<td>8 l 2'..</td>
<td>0,1/2,z [u,v,0]</td>
<td>1/2,0,z [v,u,0]</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
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<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
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</tr>
<tr>
<td>4 g 4..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<tr>
<td>4 f 2'/m..</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
<td>4 e 2'/m'..</td>
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<td>1/2,0,0 [v,u,0]</td>
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<tr>
<td>2 d 4'/m..</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2 c 4'/m'..</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>2 b 4/m..</td>
<td>0,0,1/2 [0,0,w]</td>
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<tr>
<td>2 a 4/m'..</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p_p 4  
  \[ \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \]
  Origin at 0,0,z

- Along [1,0,0] p2mm1'  
  \[ \mathbf{a}^* = \mathbf{b}, \mathbf{b}^* = \mathbf{c} \]
  Origin at x,0,0

- Along [1,1,0] p222 2m'm'  
  \[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2, \mathbf{b}^* = \mathbf{c} \]
  Origin at x,x,0
Origin at center (2/m) on 4_2

Asymmetric unit \[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2} \]

Symmetry Operations

1. \[ 1 \]
2. \[ 2 \quad 0,0,z \]
\[ (2_2) \quad 0,0,0 \]
3. \[ 4^z (0,0,1/2) \quad 0,0,z \]
\[ (4_z) \quad 0,0,1/2 \]
4. \[ 1 \]
5. \[ 1 \]
\[ (1|0,0,0) \]
6. \[ m \quad x,y,0 \]
\[ (m_z) \quad 0,0,0 \]
7. \[ 4^{x} (0,0,z) \quad 0,0,1/4 \]
\[ (4_z) \quad 0,0,1/2 \]
8. \[ 4^z (0,0,z) \quad 0,0,1/4 \]
\[ (4^{x}_z) \quad 0,0,1/2 \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

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<thead>
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<th>Coordinates</th>
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<tr>
<td>8 k 1</td>
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</tr>
<tr>
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<td>(2) ( \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}] )</td>
</tr>
<tr>
<td></td>
<td>(3) ( \bar{y}, x, z + 1/2 [\bar{v}, u, w] )</td>
</tr>
<tr>
<td></td>
<td>(4) ( y, \bar{x}, z + 1/2 [v, u, \bar{w}] )</td>
</tr>
<tr>
<td></td>
<td>(5) ( \bar{x}, \bar{y}, \bar{z} [u, v, w] )</td>
</tr>
<tr>
<td>4 j m..</td>
<td>x,y,0 [0,0,w]</td>
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<tr>
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<td>( x, \bar{y}, 0 [0,0,w] )</td>
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<tr>
<td></td>
<td>( \bar{y}, x, 1/2 [0,0,w] )</td>
</tr>
<tr>
<td></td>
<td>y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 i 2..</td>
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</tr>
<tr>
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<td>1/2,0,z + 1/2 [0,0,w]</td>
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<td>1/2,1/2,3/4 [0,0,w]</td>
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<td>2 e 4..</td>
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<tr>
<td>2 c 2/m..</td>
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<td>1/2,0,1/2 [0,0,w]</td>
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<tr>
<td>2 b 2/m..</td>
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</tbody>
</table>

2/f 4..  \( \bar{a}, \bar{b}, \bar{c} \)

Symmetry of Special Projections

Along [0,0,1] p41'
\( a^* = \bar{a}, \ b^* = \bar{b}, \ c^* = \bar{c} \)
Origin at 0,0,z

Along [1,0,0] p2'mm'
\( a^* = -c, \ b^* = \bar{b}, \ c^* = \bar{c} \)
Origin at x,0,0

Along [1,1,0] p2'mm'
\( a^* = -c, \ b^* = (-\bar{a} + \bar{b})/2 \)
Origin at x,x,0
Origin at center (2/m1') on 421'

Asymmetric unit  
\(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For 1 + set

1. \((1,0,0,0)\)
2. \((2,0,0,z)\)
3. \((3,4^*,0,0,1/2,0,0,z)\)
4. \((4,4^-,0,0,1/2,0,0,z)\)

For 1' + set

1. \((1',0,0,0)\)
2. \((2',0,0,z)\)
3. \((3,4'^*,0,0,1/2,0,0,z)\)
4. \((4,4'^-,0,0,1/2,0,0,z)\)
Continued

84.2.714  P4\_1/m1'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

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<th>Positions</th>
<th>Coordinates</th>
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<td>(5) x,y,z [0,0,0]</td>
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<td>(6) x,y,z [0,0,0]</td>
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<td>(7) y,x,z+1/2 [0,0,0]</td>
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<td>(8) y,x,z+1/2 [0,0,0]</td>
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<td>x,y,0 [0,0,0]</td>
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<td>y,x,1/2 [0,0,0]</td>
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<td>y,x,1/2 [0,0,0]</td>
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<td>2  c  2/m..1'</td>
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<td>2  b  2/m..1'</td>
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Symmetry of Special Projections

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<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p41'</th>
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<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
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<td>Origin at 0,0,z</td>
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<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = c</td>
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<td>Origin at x,0,0</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
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</tbody>
</table>
Origin at center (2/m) on 4\_2\,'

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2} \]

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(1|0,0,0) & \quad (2) & \quad 2 \quad 0,0,z \\
& & (2_z|0,0,0) & \quad (3) & \quad 4^{+} \cdot (0,0,1/2) \quad 0,0,z \\
& & & & (4_z|0,0,1/2) \quad (4) & \quad 4^{-} \cdot (0,0,1/2) \quad 0,0,z \\
& & & & (4_z^{-1}|0,0,1/2) \quad (5) & \quad \overline{1} \quad 0,0,0 \\
(1|0,0,0) & \quad (6) & \quad m \quad x,y,0 \\
& & (m_z|0,0,0) & \quad (7) & \quad \overline{4}^{+} \cdot 0,0,z; 0,0,1/4 \\
& & & & (4_z|0,0,1/2) \quad (8) & \quad \overline{4}^{-} \cdot 0,0,z; 0,0,1/4 \\
& & & & (4_z^{-1}|0,0,1/2) \end{align*}
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>( x, y, z )</th>
<th>( x, y, z )</th>
<th>( y, x, z + 1/2 )</th>
<th>( y, x, z + 1/2 )</th>
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<td>( x, y, z [u,v,w] )</td>
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<tr>
<td>8 k</td>
<td>(5) ( x, y, z ) [u,v,w]</td>
<td>( x, y, z ) [u,v,w]</td>
<td>( y, x,z+1/2 [v,u,w] )</td>
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<tr>
<td>4 j m..</td>
<td>x,y,0 [0,0,w]</td>
<td>( x, y,0 [0,0,w] )</td>
<td>( y, x,1/2 [0,0,w] )</td>
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<td>1/2,1/2,0 [0,0,w]</td>
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<td>4 g 2..</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0+1/2 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0+1/2 [0,0,w]</td>
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<tr>
<td>2 f 4'..</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
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<td>0,0,1/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
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<td>1/2,0,0 [0,0,w]</td>
<td>0,1/2,1/2 [0,0,w]</td>
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<tr>
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<td>0,1/2,0 [0,0,w]</td>
<td>1/2,0,1/2 [0,0,w]</td>
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<td>1/2,0,1/2 [0,0,w]</td>
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<tr>
<td>2 b 2/m..</td>
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<td>1/2,1/2,1/2 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
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</table>

### Symmetry of Special Projections

- **Along \([0,0,1]\) p41'**
  - \( a^* = a \) \( b^* = b \)
  - Origin at 0,0,z

- **Along \([1,0,0]\) p2'\(\text{mm}'\)**
  - \( a^* = -c \) \( b^* = b \)
  - Origin at x,0,0

- **Along \([1,1,0]\) p2'\(\text{mm}'\)**
  - \( a^* = -c \) \( b^* = (-a + b)/2 \)
  - Origin at x,x,0
Origin at center (2/m') on 4₂

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1|0,0,0) \\
(2) & \quad 2, 0,0,z \\
& \quad (2z|0,0,0) \\
(3) & \quad 4^* (0,0,1/2), 0,0,z \\
& \quad (4z|0,0,1/2) \\
(4) & \quad 4^* (0,0,1/2), 0,0,z \\
& \quad (4z^{-1}|0,0,1/2) \\
(5) & \quad \bar{1}^*, 0,0,0 \\
& \quad (1|0,0,0)' \\
(6) & \quad m', x,y,0 \\
& \quad (mz|0,0,0) \\
(7) & \quad \bar{4}^* (0,0,z); 0,0,1/4 \\
& \quad (4z|0,0,1/2)' \\
(8) & \quad \bar{4}^* (0,0,z); 0,0,1/4 \\
& \quad (4z^{-1}|0,0,1/2)'
\end{align*}
\]
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<td>1/2,1/2,1/4 [0,0,0]</td>
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<td>1/2,1/2,3/4 [0,0,0]</td>
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<td>0,0,3/4 [0,0,0]</td>
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<td>2 d 2/m'..</td>
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<td>1/2,0,0 [0,0,0]</td>
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</table>

### Symmetry of Special Projections

**Along [0,0,1] p4**  
\( a^* = a \)  
\( b^* = b \)

**Origin at 0,0,z**

**Along [1,0,0] p2m'**  
\( a^* = b \)  
\( b^* = c \)

**Origin at x,0,0**

**Along [1,1,0] p2m'**  
\( a^* = (-a + b)/2 \)  
\( b^* = c \)

**Origin at x,x,0**
Origin at center (2/m') on 42'.

Asymmetric unit: 
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations:

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(3) 4' ' (0,0,1/2) 0,0,z
(4z|0,0,1/2)

(4') 4' ' (0,0,1/2) 0,0,z
(4z-1|0,0,1/2)

(5) 1* 0,0,0
(1|0,0,0)'

(6) m' x,y,0
(mz|0,0,0)'

(7) 4' ' 0,0,z; 0,0,1/4
(4z|0,0,1/2)

(8) 4' ' 0,0,z; 0,0,1/4
(4z-1|0,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<td>(2) x̅,y̅,z [u̅,v̅,w̅]</td>
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<td>(5) x̅,y̅,z [u̅,v̅,w̅]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(7) y,x̅,z+1/2 [v,u̅,w̅]</td>
<td>(8) y,x̅,z+1/2 [v,u̅,w̅]</td>
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<td>4 j m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>x̅,y̅,0 [u̅,v̅,0]</td>
<td>y,x,1/2 [v,u̅,0]</td>
</tr>
<tr>
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<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>0,1/2, z [0,0,w̅]</td>
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<td>1/2,1/2, z̅ [0,0,w]</td>
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<td>4 g 2..</td>
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<td>0,0,z+1/2 [0,0,w̅]</td>
<td>0,0, z̅ [0,0,w̅]</td>
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<td>2 c 2/m'..</td>
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<td>0,1/2,0 [0,0,0]</td>
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<td>2 b 2/m'..</td>
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<td>0,0,1/2 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
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</table>

### Symmetry of Special Projections

- **Along [0,0,1]** \( p4' \) \( a^* = a \) \( b^* = b \) Origin at 0,0,z
- **Along [1,0,0]** \( p2m'm' \) \( a^* = b \) \( b^* = c \) Origin at x,0,0
- **Along [1,1,0]** \( p2m'm' \) \( a^* = (-a + b)/2 \) \( b^* = c \) Origin at x,x,0
Origin at center (2/m) on \(4_2\)

Asymmetric unit: 

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

For \((0,0,0)\) + set

1. 1
2. 2 \((0,0,0)\), \(2z\) \((0,0,0)\)
3. \(4^+ (0,0,1/2)\) \(0,0,z\) \((4z)0,0,1/2\)
4. \(4^- (0,0,1/2)\) \(0,0,z\) \((4z)^{-1}0,0,1/2\)
5. \(m\) \(x,y,0\) \((mz)0,0,0\)
6. \(4^* (0,0,1/4)\) \(0,0,1/4\) \((4z)0,0,1/4\)
7. \(4^- (0,0,1/4)\) \(0,0,1/4\) \((4z)^{-1}0,0,1/4\)

For \((1,0,0)\)' + set

1. \((1,0,0)\)'\(1,0,0)\)
2. \(2' 1/2,0,z\) \((2z)1,0,0)\)
3. \(4' (0,0,1/2)\) \(1/2,1/2,z\) \((4z)1,0,1/2)\)
4. \(4' (0,0,1/2)\) \(1/2,-1/2,z\) \((4z)^{-1}1,0,1/2)\)
5. \((1,0,0)\)'\(1/2,0,0\)
6. \(a' (1,0,0)\) \(x,y,0\) \((mz)1,0,0)\)
7. \(4' (0,0,1/2)\) \(1/2,-1/2,z\) \((4z)1,0,1/2)\)
8. \(4' (0,0,1/2)\) \(1/2,1/2,z\) \((4z)^{-1}1,0,1/2)\)
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>(1,0,0)' +</td>
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<td>8 2'</td>
<td>0,1/2,z [u,v,0] 1/2,0,z+1/2 [v,u,0] 0,1/2,z [u,v,0] 1/2,0,z+1/2 [v,u,0]</td>
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<td>4 2'</td>
<td>0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0]</td>
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<td>4 2</td>
<td>0,0,0 [0,0,w] 0,0,1/2 [0,0,w]</td>
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Symmetry of Special Projections

Along [0,0,1]  p41'  Along [1,0,0]  p2mm1'  Along [1,1,0]  p2c2 2mm

a* = a  b* = b  a* = b  b* = b  a* = (-a + b)/2  b* = c

Origin at 0,0,z  Origin at x,0,0  Origin at x-1/4,x+1/4,0
Origin at center (2/m') on 4₂

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 
(1 0 0,0)

(2) 2 0,0,z
(2z 0,0,0)

(3) 4⁺ (0,0,1/2) 0,0,z
(4z 0,0,1/2)

(4) 4⁻ (0,0,1/2) 0,0,z
(4z⁻¹ 0,0,1/2)

(5) T⁺ 0,0,0
(1 0,0,0)'

(6) m' x,y,0
(mz 0,0,0)'

(7) 4⁻⁺⁺ 0,0,z; 0,0,1/4
(4z 0,0,1/2)'

(8) 4⁻⁻⁻ 0,0,z; 0,0,1/4
(4z⁻¹ 0,0,1/2)'

For (1,0,0) + set

(1) t⁺ (1,0,0)
(1 1,0,0)'

(2) 2' 1/2,0,z
(2z 1,0,0)'

(3) 4⁺⁺ (0,0,1/2) 1/2,1/2,z
(4z 1,0,1/2)'

(4) 4⁻⁺ (0,0,1/2) 1/2,-1/2,z
(4z⁻¹ 1,0,1/2)'

(5) T 1/2,0,0
(T 1,0,0)

(6) a (1,0,0) x,y,0
(mz 1,0,0)

(7) 4⁺⁻ (1/2,-1/2,z; 1/2,-1/2,1/4
(4z 1,0,1/2)

(8) 4⁻⁻⁻ (1/2,1/2,z; 1/2,1/2,1/4
(4z⁻¹ 1,0,1/2)

Continued
### Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<tr>
<td>4 a</td>
<td>2/m'</td>
<td>(0,0,0)</td>
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### Symmetry of Special Projections

- **Along [0,0,1]**  \( p_p \cdot 4 \)  
  - \( a^* = a \)
  - \( b^* = b \)

- **Along [1,0,0]**  \( p_{2mm1} \)  
  - \( a^* = b \)
  - \( b^* = c \)

- **Along [1,1,0]**  \( p_{2m} \cdot 2m' \)  
  - \( a^* = (a+b)/2 \)
  - \( b^* = c \)
Origin at \( \bar{1} \) on \( n \), -1/4,1/4,0 from \( \bar{1} \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

Symmetry Operations

1. \( 1 \)
   \[ (1 | 0,0,0) \]

2. \( 2 \) \( 0,0,z \)
   \[ (2_z | 0,0,0) \]

3. \( 4^+ \) \( 0,1/2,z \)
   \[ (4_z | 1/2,1/2,0) \]

4. \( 4^* \) \( 1/2,0,z \)
   \[ (4_{z^1} | 1/2,1/2,0) \]

5. \( \bar{T} \) \( 1/4,1/4,0 \)
   \[ (1 | 1/2,1/2,0) \]

6. \( n \) \( (1/2,1/2,0) \) \( x,y,0 \)
   \[ (m_z | 1/2,1/2,0) \]

7. \( 4^* \) \( 0,0,z \)
   \[ (4_z | 0,0,0) \]

8. \( 4^* \) \( 0,0,z \)
   \[ (4_{z^1} | 0,0,0) \]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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Symmetry of Special Projections

Along [0,0,1]   p4          Along [1,0,0]   p2mg'          Along [1,1,0]   p2mm
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z  Origin at x,1/4,0  Origin at x,x,0
Origin at $\overline{1'}$ on $n$, -1/4, 1/4, 0 from $\overline{1'}$

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$

Symmetry Operations

1 + set

(1) 1
   (1 | 0,0,0)

(2) 2 $\overline{0,0,z}$
   ($2_{z} | 0,0,0$)

(3) $4^{+} 0,1/2,z$
   ($4_{z} | 1/2,1/2,0$)

(4) $4^{+} 1/2,0,z$
   ($4_{z}^{-1} | 1/2,1/2,0$)

(5) $\overline{1}/4,1/4,0$
   ($\overline{1} | 1/2,1/2,0$)

(6) n $1/2,1/2,0$ x,y,0
   ($m_{z} | 1/2,1/2,0$)

(7) $\overline{4}^{+} 0,0,z; 0,0,0$
   ($\overline{4}_{z} | 0,0,0$)

(8) $\overline{4}^{+} 0,0,z; 0,0,0$
   ($\overline{4}_{z}^{-1} | 0,0,0$)

1' + set

(1) 1'
   (1 | 0,0,0')

(2) 2' $\overline{0,0,z}$
   ($2_{z} | 0,0,0'$)

(3) $4^{+} 0,1/2,z$
   ($4_{z} | 1/2,1/2,0'$)

(4) $4^{-} 1/2,0,z$
   ($4_{z}^{-1} | 1/2,1/2,0'$)

(5) $\overline{1}/4,1/4,0$
   ($\overline{1} | 1/2,1/2,0'$)

(6) n' $1/2,1/2,0$ x,y,0
   ($m_{z} | 1/2,1/2,0'$)

(7) $\overline{4}^{+} 0,0,z; 0,0,0$
   ($\overline{4}_{z} | 0,0,0'$)

(8) $\overline{4}^{-} 0,0,z; 0,0,0$
   ($\overline{4}_{z}^{-1} | 0,0,0'$)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
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<tr>
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<tr>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'  
\( a^* = (a - b)/2 \)  
\( b^* = (a + b)/2 \)  
Origin at 0,0,z

Along [1,0,0] p2mg1'  
\( a^* = b \)  
\( b^* = c \)  
Origin at x,1/4,0

Along [1,1,0] p2mm1'  
\( a^* = (-a + b)/2 \)  
\( b^* = c \)  
Origin at x,x,0
Origin at $\overline{4}$ on n, -1/4,1/4,0 from 1

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

1. $\{1\} (1|0,0,0)$
2. $\{2\} 0,0,z (2z|0,0,0)$
3. $\{4\} 0,1/2,z (4z|1/2,1/2,0)'$
4. $\{4\} 1/2,0,z (4z'^{-1}|1/2,1/2,0)'$
5. $\{\overline{1}\} 1/4,1/4,0 (\overline{1}|1/2,1/2,0)$
6. $n (1/2,1/2,0) x,y,0 (m|1/2,1/2,0)$
7. $\overline{4} 0,0,z; 0,0,0 (4z|0,0,0)'$
8. $\overline{4} 0,0,z; 0,0,0 (4z'^{-1}|0,0,0)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<tr>
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<tr>
<td>4 f 2..</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 1</td>
<td>1/4,1/4,1/2 [u,v,w]</td>
<td>3/4,3/4,1/2 [v,u,w]</td>
<td>1/4,3,1/2 [v,u,w]</td>
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<td>2 c 4'..</td>
<td>0,1/2,z [0,0,0]</td>
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<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'Along [1,0,0] p2'm'gAlong [1,1,0] p2mm
\[a^* = (a - b)/2\] \[b^* = (a + b)/2\] \[a^* = b \] \[b^* = c\] \[a^* = -(a + b)/2\] \[b^* = c\]
Origin at 0,0,z Origin at x,1/4,0 Origin at x,x,0
**Origin** at \( \overline{4} \) on \( n' \), -1/4,1/4,0 from \( \overline{1}' \)

**Asymmetric unit**  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

<table>
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<th>No.</th>
<th>Operation</th>
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<td>1</td>
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<tr>
<td>2</td>
<td>2 ( 0,0,z )</td>
<td>( (2_z</td>
</tr>
<tr>
<td>3</td>
<td>4 ( 0,1/2,z )</td>
<td>( (4_z</td>
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<tr>
<td>4</td>
<td>4 ( 1/2,0,z )</td>
<td>( (4_z'^{-1}</td>
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<tr>
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<td>( b ) ( 1/4,1/4,0 )</td>
<td>( (b</td>
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<td>6</td>
<td>( n' ) ( (1/2,1/2,0) )</td>
<td>( (n'</td>
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<tr>
<td>7</td>
<td>( 4^{+} ) ( 0,0,z )</td>
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<tr>
<td>8</td>
<td>( 4^{-} ) ( 0,0,z )</td>
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Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

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| 4 f 2.. 0,0,z [0,0,w]                     | 1/2,1/2,z [0,0,w] |
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| 2 c 4.. 0,1/2,z [0,0,w]                  | 1/2,0,z [0,0,w] |
| 2 b 4.. 0,0,1/2 [0,0,0]                  | 1/2,1/2,1/2 [0,0,0] |
| 2 a 4.. 0,0,0 [0,0,0]                    | 1/2,1/2,0 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p_4. 4  
Along [1,0,0] p2m'g'  
Along [1,1,0] p2m'm'

a* = (a - b)/2  
b* = (a + b)/2  
a* = b  
b* = c

Origin at 1/2,0,z  
Origin at x,1/4,0  
Origin at x,x,0

85.4.723 - 2 - 1439
**Origin** at $\bar{4}$ on $n'$, $-1/4,1/4,0$ from $\bar{1}'$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

1. $1$
   
   $(1|0,0,0)$

2. $2$ 0,0,z
   
   $(2_z|0,0,0)$

3. $4' \cdot 0,1/2,z$
   
   $(4_z|1/2,1/2,0)'$

4. $4' \cdot 1/2,0,z$
   
   $(4_z^{-1}|1/2,1/2,0)'$

5. $\bar{1}'$ 1/4,1/4,0
   
   $(1|1/2,1/2,0)'$

6. $n'$ (1/2,1/2,0) x,y,0
   
   $(m_z|1/2,1/2,0)'$

7. $4' \cdot 0,0,z; 0,0,0$
   
   $(4_z|0,0,0)$

8. $4' \cdot 0,0,z; 0,0,0$
   
   $(4_z^{-1}|0,0,0)$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<tr>
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<tr>
<td></td>
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</table>

Symmetry of Special Projections

Along [0,0,1] \(p_\rho,4\) \(a^* = (a - b)/2\) \(b^* = (a + b)/2\) Origin at 0,0,z
Along [1,0,0] \(p2m'g'\) \(a^* = b\) \(b^* = c\) Origin at x,1/4,0
Along [1,1,0] \(p2m'm'\) \(a^* = (-a + b)/2\) \(b^* = c\) Origin at x,x,0
Origin at \( \bar{4} \) on \(-1/4,1/4,0\) from \(1\)

Asymmetric unit \(0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
2. \(2\) \(0,0,z\)
3. \(4^+\) \(0,1/2,z\)
4. \(4\) \(1/2,0,z\)
5. \(T\) \(1/4,1/4,0\)
6. \(n\) \((1/2,1/2,0)\) \(x,y,0\)
7. \(4^+\) \(0,0,z; 0,0,0\)
8. \(4\) \(-1/2,1/2,0\)

For \((0,0,1)\)' + set

1. \(t'\) \((0,0,1)\)
2. \(2'\) \((0,0,1)'\) \(0,0,z\)
3. \(4'^+\) \((0,0,1)'\) \(0,1/2,1,2,1)'\)
4. \(4'\) \((0,0,1)\) \(1/2,0,z\)
5. \(T'\) \(1/4,1/4,1/2\)
6. \(n'\) \((1/2,1/2,0)\) \(x,y,1/2\)
7. \(4'^+\) \(0,0,z; 0,0,1/2\)
8. \(4'\) \(-1/2,1/2,1)'

85.6.725 - 1 - 1442
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' +</td>
<td></td>
</tr>
</tbody>
</table>

16 g  1  (1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y+1/2,x+1/2,z [v,u,w]  (4) y+1/2,x+1/2,z [v,u,w]  (5) x+1/2,y+1/2,z [u,v,w]  (6) x+1/2,y+1/2,z [u,v,w]  (7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]

8 f 2.. 0,0,z [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]  0,0,z [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]  0,0,z [0,0,w]

8 e 1/4,1/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]

8 d 1/4,1/4,0 [u,v,w]  3/4,3/4,0 [v,u,w]  1/4,3/4,0 [v,u,w]  3/4,1/4,0 [v,u,w]  1/4,3/4,0 [v,u,w]  3/4,1/4,0 [v,u,w]  3/4,1/4,0 [v,u,w]  3/4,1/4,0 [v,u,w]

4 c 4.. 0,1/2,z [0,0,w]  1/2,0,z [0,0,w]  1/2,0,z [0,0,w]  0,1/2,z [0,0,w]  1/2,0,z [0,0,w]  1/2,0,z [0,0,w]  0,1/2,z [0,0,w]  1/2,0,z [0,0,w]

4 b 4'.. 0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]

4 a 4'.. 0,0,0 [0,0,w]  1/2,1/2,0 [0,0,w]  1/2,1/2,0 [0,0,w]  0,0,0 [0,0,w]  1/2,1/2,0 [0,0,w]  1/2,1/2,0 [0,0,w]  0,0,0 [0,0,w]  1/2,1/2,0 [0,0,w]

Symmetry of Special Projections

Along [0,0,1]  p41'  Along [1,0,0]  p2a' 2m'g'  Along [1,1,0]  p2a' 2m'm'

a* = (a - b)/2  b* = (a + b)/2  a* = b  b* = c  a* = -c  b* = (-a + b)/2

Origin at 0,0,z  Origin at x,1/4,1/2  Origin at x,1/4,1/2
Origin at $\bar{4}$ on $n$, $-1/4,1/4,0$ from $\bar{1}$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

(1) $1$

(1) $0,0,0$

(2) $2$ $0,0,z$

(2) $0,0,0$

(3) $4^+ \cdot 0,1/2,z$

(4) $4^- \cdot 0,0,z$

(4) $1/2,0,z$

(4) $1/2,0,z$

(5) $\bar{1} 1/4,1/4,0$

(5) $1/2,1/2,0$

(6) $n$ $(1/2,1/2,0)$ $x,y,0$

(6) $m_z$ $(1/2,1/2,0)$

(7) $\bar{4}^+ \cdot 0,0,z$; $0,0,0$

(7) $\bar{4}^- \cdot 0,0,z$; $0,0,0$

(7) $0,0,0$

(7) $0,0,0$

For $(0,0,1')$ + set

(1) $t'$ $(0,0,1)$

(1) $0,0,1'$

(2) $2'$ $(0,0,1)$ $0,0,z$

(2) $0,0,1'$

(3) $4^+ (0,0,1)$ $0,1/2,z$

(4) $4^- (0,0,1)$ $0,0,1/2$

(3) $0,1/2,0,z$

(4) $0,0,1/2$

(4) $1/2,0,z$

(4) $1/2,0,z$

(5) $\bar{1}' 1/4,1/4,1/2$

(5) $1/2,1/2,1'$

(6) $n'$ $(1/2,1/2,0)$ $x,y,1/2$

(6) $m_z$ $(1/2,1/2,1)'$

(7) $\bar{4}^+ 0,0,z$; $0,0,1/2$

(7) $\bar{4}^- 0,0,z$; $0,0,1/2$

(8) $\bar{4}^- 0,0,z$; $0,0,1/2$

(8) $\bar{4}^- 0,0,z$; $0,0,1/2$

85.7.726 - 1 - 1444
Continued 85.7.726

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
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</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x̅,y̅,z [u̅,v̅,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,w]</td>
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<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,1/2 [0,0,0]</td>
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<td>1/4,3/4,1/2 [0,0,0]</td>
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<td>3/4,1/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 d</td>
<td>1/4,1/4,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,0 [v,u,w]</td>
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<td></td>
<td>1/4,3/4,0 [v,u,w]</td>
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<td></td>
<td>3/4,1/4,0 [v,u,w]</td>
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<tr>
<td>4 c</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4₁'  
\[ \mathbf{a^*} = (\mathbf{a} - \mathbf{b})/2 \  \mathbf{b^*} = (\mathbf{a} + \mathbf{b})/2 \]

Origin at 0,0,z

Along [1,0,0] p₂₄* 2m'g'  
\[ \mathbf{a^*} = \mathbf{b} \  \mathbf{b^*} = \mathbf{c} \]

Origin at x,1/4,1/2

Along [1,1,0] p₂₄* 2m'm'  
\[ \mathbf{a^*} = -\mathbf{c} \  \mathbf{b^*} = (-\mathbf{a} + \mathbf{b})/2 \]

Origin at x,x,1/2

85.7.726 - 2 - 1445
**Origin** at \( \overline{4} \) at \(-1/4, -1/4, -1/4\) from \( \overline{1} \)

**Asymmetric unit** \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

**Symmetry Operations**

1. \( 1 \)
   - \( (1|0,0,0) \)
2. \( 2 \)
   - \( 0,0,z \)
   - \( (2_z|0,0,0) \)
3. \( 4^+ \)
   - \( (0,0,1/2); 0,1/2,z \)
   - \( (4_z|1/2,1/2,1/2) \)
   - \( (4_z^{-1}|1/2,1/2,1/2) \)
4. \( 4^- \)
   - \( (0,0,1/2); 1/2,0,z \)
   - \( (4_z|1/2,1/2,1/2) \)
   - \( (4_z^{-1}|1/2,1/2,1/2) \)
5. \( \overline{1} \)
   - \( 1/4,1/4,1/4 \)
   - \( (1|1/2,1/2,1/2) \)
   - \( (1/2,1/2,1/2) \)
6. \( n \)
   - \( (1/2,1/2,0); x,y,1/4 \)
   - \( (m_z|1/2,1/2,1/2) \)
7. \( 4^* \)
   - \( 0,0,z; 0,0,0 \)
   - \( (4_z|0,0,0) \)
8. \( 4^* \)
   - \( 0,0,z; 0,0,0 \)
   - \( (4_z|0,0,0) \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>8 g 1 (1) x,y,z [u,v,w]</td>
<td>( \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}] )</td>
</tr>
<tr>
<td>(3) ( \bar{y}+1/2,x+1/2,z+1/2 ) ([\bar{v},u,w])</td>
<td>( y+1/2,\bar{x}+1/2,z+1/2 ) ([v,\bar{u},w])</td>
</tr>
<tr>
<td>(5) ( \bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2 ) ([u,v,w])</td>
<td>( x+1/2,y+1/2,\bar{z}+1/2 ) ([\bar{u},v,w])</td>
</tr>
<tr>
<td>(7) ( y,\bar{x},\bar{z} ) ([v,u,w])</td>
<td>( \bar{y},x,\bar{z} ) ([v,u,w])</td>
</tr>
<tr>
<td>4 f 2.. 0,0,z [0,0,w]</td>
<td>( 1/2,1/2,z+1/2 ) ([0,0,w])</td>
</tr>
<tr>
<td>4 e 2.. 0,1/2,z [0,0,w]</td>
<td>( 0,1/2,z+1/2 ) ([0,0,w])</td>
</tr>
<tr>
<td>4 d ( \bar{a} ) 1/4,1/4,3/4 ([u,v,w])</td>
<td>( 3/4,3/4,1/4 ) ([\bar{u},v,w])</td>
</tr>
<tr>
<td>4 c ( \bar{a} ) 1/4,1/4,1/4 ([u,v,w])</td>
<td>( 3/4,3/4,3/4 ) ([\bar{u},v,w])</td>
</tr>
<tr>
<td>2 b ( \bar{a} ) 0,0,1/2 [0,0,w]</td>
<td>( 1/2,1/2,0 ) ([0,0,w])</td>
</tr>
<tr>
<td>2 a ( \bar{a} ) 0,0,0 [0,0,w]</td>
<td>( 1/2,1/2,1/2 ) ([0,0,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along \([0,0,1]\) p4  
  \( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  
- Along \([1,0,0]\) p2'm'g  
  \( a^* = b \)  \( b^* = c \)  
- Along \([1,1,0]\) p2'm'm'g  
  \( a^* = -c \)  \( b^* = (-a + b)/2 \)

Origin at 0,0,z  
Origin at x,1/4,1/4  
Origin at x,x,1/4
Origin at \( \bar{4} 1' \) at \(-1/4,-1/4,-1/4\) from \( \bar{1} 1' \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

For \( 1 + \) set

- **(1)** \( 1 \) (1 0 0,0)
  - (2) \( 2 \) 0,0,z
  - \( (2_z 0,0,0) \)
  - (3) \( 4^* 0,0,1/2 \) 0,1/2,z
  - \( (4_z 1/2,1/2,1/2) \)
  - (4) \( 4' 0,0,1/2 \) 1/2,0,z
  - \( (4_z^{-1} 1/2,1/2,1/2) \)
- **(5)** \( \bar{1} 1/4,1/4,1/4 \) (1 1/2,1/2,1/2)
  - (6) \( n (1/2,1/2,0) x,y,1/4 \)
  - \( (m_z 1/2,1/2,1/2) \)
  - (7) \( \bar{4}^* 0,0,z; 0,0,0 \)
  - \( (4_z 0,0,0) \)
  - (8) \( \bar{4} \) 0,0,z; 0,0,0
  - \( (4_z^{-1} 0,0,0) \)

For \( 1' + \) set

- **(1)** \( 1' \) (1 0 0,0')
  - (2) \( 2' 0,0,z \)
  - \( (2_z 0,0,0)' \)
  - (3) \( 4'^* 0,0,1/2 \) 0,1/2,z
  - \( (4_z 1/2,1/2,1/2)' \)
  - (4) \( 4'\) 0,0,1/2 \) 1/2,0,z
  - \( (4_z^{-1} 1/2,1/2,1/2)' \)
- **(5)** \( \bar{1}' 1/4,1/4,1/2 \) (1 1/2,1/2,1/2')
  - (6) \( n' (1/2,1/2,0) x,y,0 \)
  - \( (m_z 1/2,1/2,1/2)' \)
  - (7) \( \bar{4}'^* 0,0,z; 0,0,0 \)
  - \( (4_z 0,0,0)' \)
  - (8) \( \bar{4}' \) 0,0,z; 0,0,0
  - \( (4_z^{-1} 0,0,0)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
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<tr>
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<tbody>
<tr>
<td>Coordinates</td>
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<tr>
<td>1 + 1' +</td>
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</table>

<table>
<thead>
<tr>
<th>8 g 11'</th>
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<tbody>
<tr>
<td>1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>2) (\bar{x},\bar{y},z) [0,0,0]</td>
</tr>
<tr>
<td>3) (\bar{y}+1/2,x+1/2,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td>4) (y+1/2,\bar{x}+1/2,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td>5) (\bar{x}+1/2,\bar{y}+1/2,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td>6) (x+1/2,y+1/2,\bar{z}+1/2) [0,0,0]</td>
</tr>
<tr>
<td>7) (y,\bar{x},z) [0,0,0]</td>
</tr>
<tr>
<td>8) (\bar{y},x,z) [0,0,0]</td>
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<tr>
<th>4 f 2...1'</th>
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</thead>
<tbody>
<tr>
<td>0,0,z [0,0,0]</td>
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<tr>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>1/2,1/2,\bar{z}+1/2 [0,0,0]</td>
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<tr>
<td>0,0,\bar{z} [0,0,0]</td>
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<td>0.1/2,z [0,0,0]</td>
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<td>0.1/2,z+1/2 [0,0,0]</td>
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<tr>
<td>1/2,0,\bar{z}+1/2 [0,0,0]</td>
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<th>4 d (\bar{1}')</th>
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<td>1/4,1/4,3/4 [0,0,0]</td>
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<tr>
<td>3/4,3/4,3/4 [0,0,0]</td>
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<td>1/4,3/4,1/4 [0,0,0]</td>
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<td>3/4,1/4,1/4 [0,0,0]</td>
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<td>1/4,1/4,1/4 [0,0,0]</td>
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<tr>
<td>3/4,3/4,1/4 [0,0,0]</td>
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<td>3/4,1/4,3/4 [0,0,0]</td>
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<thead>
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<th>2 b (\bar{4}...1')</th>
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<tbody>
<tr>
<td>0,0,1/2 [0,0,0]</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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Symmetry of Special Projections

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<th>Along [0,0,1] p41'</th>
<th>Along [1,0,0] p2mg1'</th>
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<td>(a^* = (a-b)/2) (b^* = (a+b)/2)</td>
<td>(a^* = b) (b^* = c)</td>
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</tbody>
</table>
-Origin at 0,0,z | Origin at x,1/4,1/4|

<table>
<thead>
<tr>
<th>Along [1,1,0] p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = -(a+b)/2) (b^* = c)</td>
</tr>
</tbody>
</table>
Origin at $\bar{4}$ at $-1/4,-1/4,-1/4$ from $\bar{1}$

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations:

1. $1$
   \( (1|0,0,0) \)

2. $2$ 0,0,z
   \( (2|0,0,0) \)

3. $4^{-}$ (0,0,1/2) 0,1/2,z
   \( (4_{z}|1/2,1/2,1/2) \)

4. $4^{-}$ (0,0,1/2) 1/2,0,z
   \( (4_{z}^{-1}|1/2,1/2,1/2) \)

5. $\bar{4}$ 1/4,1/4,1/4
   \( (\bar{1}|1/2,1/2,1/2) \)

6. n (1/2,1/2,0) x,y,1/4
   \( (m_{z}|1/2,1/2,1/2) \)

7. $4^{-}$ 0,0,z; 0,0,0
   \( (4_{z}|0,0,0) \)

8. $\bar{4}$ 0,0,z; 0,0,0
   \( (\bar{4}_{z}|0,0,0) \)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<tr>
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<td>(4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
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| 4 f 2..      | 0,0,z [0,0,0] |
|              | 1/2,1/2,z+1/2 [0,0,0] |
|              | 1/2,1/2,z+1/2 [0,0,0] |
|              | 0,0,z [0,0,0] |

| 4 e 2..      | 0,1/2,z [0,0,0] |
|              | 1/2,0,z+1/2 [0,0,0] |
|              | 1/2,0,z+1/2 [0,0,0] |
|              | 0,1/2,z [0,0,0] |

| 4 d 1/2..    | 1/4,1/4,3/4 [u,v,w] |
|              | 3/4,3/4,3/4 [u,v,w] |
|              | 3/4,3/4,1/4 [v,u,w] |
|              | 1/4,3/4,1/4 [v,u,w] |

| 4 c 1/2..    | 1/4,1/4,1/4 [u,v,w] |
|              | 1/4,3/4,1/4 [v,u,w] |
|              | 3/4,1/4,3/4 [v,u,w] |

| 2 b 1/2..    | 0,0,1/2 [0,0,0] |
|              | 1/2,1/2,0 [0,0,0] |

| 2 a 1/2..    | 0,0,0 [0,0,0] |
|              | 1/2,1/2,1/2 [0,0,0] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = (a - b)/2$</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2'm'g</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = b$</td>
<td></td>
</tr>
<tr>
<td>$b^* = c$</td>
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<tr>
<td>Origin at x,1/4,1/4</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = -c$</td>
<td></td>
</tr>
<tr>
<td>$b^* = (-a + b)/2$</td>
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<tr>
<td>Origin at x,x,1/4</td>
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</tbody>
</table>
Origin at $\bar{1}^*$ at -1/4,-1/4,-1/4 from $\bar{1}^*$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $1$
2. $2 \begin{pmatrix} 0,0,z \\ (2_z) \end{pmatrix} \begin{pmatrix} 0,0,0 \\ 0,0,0 \\ \end{pmatrix}$
3. $4^* \begin{pmatrix} 0,0,1/2; 0,1/2,z \\ (4_z) \end{pmatrix} \begin{pmatrix} 0,1/2,1/2,1/2 \\ 1/2,0,z \\ \end{pmatrix}$
4. $4^- \begin{pmatrix} 0,0,1/2; 1/2,0,z \\ (4_z) \end{pmatrix} \begin{pmatrix} 0,1/2,1/2,1/2 \\ 1/2,0,z \\ \end{pmatrix}$
5. $T1^* 1/4,1/4,1/4$
6. $n' \begin{pmatrix} 1/2,1/2,0; x,y,1/4 \\ (m_z) \end{pmatrix} \begin{pmatrix} 1/2,1/2,1/2 \\ 1/2,1/2,1/2 \\ \end{pmatrix}$
7. $4^{**}$ \begin{pmatrix} 0,0,z; 0,0,0 \\ (4_z) \end{pmatrix} \begin{pmatrix} 0,0,0 \\ 0,0,0 \\ \end{pmatrix}$
8. $4^* \begin{pmatrix} 0,0,0; 0,0,0 \\ (4_z) \end{pmatrix} \begin{pmatrix} 0,0,0 \\ 0,0,0 \\ \end{pmatrix}$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>(1) x,y,z [u,v,w]</td>
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<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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<tr>
<td>4</td>
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<tr>
<td>2</td>
<td>0,0,z [0,0,w]</td>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<tr>
<td>4</td>
<td>e</td>
</tr>
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<td>2</td>
<td>0,1/2,z [0,0,w]</td>
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<tr>
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<td>0,1/2,z+1/2 [0,0,w]</td>
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<td>0,1/2,z+1/2 [0,0,w]</td>
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<tr>
<td>4</td>
<td>d</td>
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<tr>
<td>1</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
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<td>3/4,3/4,1/4 [0,0,0]</td>
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<td>3/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
</tr>
<tr>
<td>1</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
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<td>3/4,3/4,1/4 [0,0,0]</td>
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<tr>
<td></td>
<td>3/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
</tr>
<tr>
<td>4</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
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<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
</tr>
<tr>
<td>4</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p, 4
a* = (a - b)/2  b* = (a + b)/2
Origin at 1/2,0,z

Along [1,0,0]  p2m'g
a* = b  b* = c
Origin at x,1/4,1/4

Along [1,1,0]  p2m'm'
a* = -(a + b)/2  b* = c
Origin at x,x,1/4
Origin at $\bar{4}$ at $-1/4, -1/4, -1/4$ from $\bar{1}'$.

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1  
(2) $2 \quad 0,0,z$  
(22) $0,0,0$  
(3) $4^{+} \cdot (0,0,1/2) \quad 0,1/2,z$  
(4) $4^{-} \cdot (0,0,1/2) \quad 1/2,0,z$  
(5) $\bar{1} \cdot 1/4,1/4,1/4$  
(6) $n' \cdot (1/2,1/2,0) \quad x,y,1/4$  
(66) $1/2,1/2,1/2$  
(7) $\bar{4}^{+} \cdot 0,0,z; \quad 0,0,0$  
(8) $\bar{4}^{-} \cdot 0,0,z; \quad 0,0,0$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
<td>4 f 2..</td>
<td>0,0,z [0,0,w]</td>
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<tr>
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<td>1/2,0,0 [0,0,w]</td>
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<tr>
<td></td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>4 d 1/4,1/4,1/4 [0,0,0]</td>
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<td>3/4,3/4,1/4 [0,0,0]</td>
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<tr>
<td>4 c 1/4,1/4,1/4 [0,0,0]</td>
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</tr>
<tr>
<td>2 b 0,0,1/2 [0,0,w]</td>
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<td>1/2,1/2,0 [0,0,w]</td>
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<tr>
<td>2 a 0,0,0 [0,0,w]</td>
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<tr>
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<td>1/2,1/2,1/2 [0,0,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] \( p_c \cdot 4 \)  
Along [1,0,0] \( p2m'g' \)  
Along [1,1,0] \( p2m'm' \)

\( a^* = (a - b)/2 \)  
\( b^* = (a + b)/2 \)  
\( a^* = b \)  
\( b^* = c \)  
\( a^* = -a + b)/2 \)  
\( b^* = c \)

Origin at 0,0,z  
Origin at x,1/4,1/4  
Origin at x,x,1/4
Origin at \( \frac{1}{4} \) at \(-1/4,-1/4,-1/4\) from \( \frac{1}{4} \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
   \((1,0,0,0)\)

2. \(2\)
   \((0,0,z)\)
   \((2z,0,0,0)\)

3. \(4^+\)
   \((0,0,1/2)\)
   \((0,1/2,z)\)
   \((4z,1/2,1/2,1/2)\)

4. \(4^-\)
   \((0,0,1/2)\)
   \((1/2,0,z)\)
   \((4z^{-1},1/2,1/2,1/2)\)

5. \(\bar{T}\)
   \((1/4,1/4,1/4)\)
   \((1/4,1/4,1/4)\)

6. \(n\)
   \((1/2,1/2,0)\)
   \((mz,1/2,1/2,1/2)\)

7. \(4^+\)
   \((0,0,z; 0,0,0)\)
   \((4z,0,0,0)\)

8. \(4^-\)
   \((0,0,z; 0,0,0)\)
   \((4z^{-1},0,0,0)\)

For \((1,0,0)'\) + set

1. \(t'\)
   \((1,0,0,0)\)'

2. \(2'\)
   \((1/2,0,z)\)
   \((2z,1,0,0)\)'

3. \(4'^+\)
   \((0,0,1/2)\)
   \((1/2,0,z)\)
   \((4z,3/2,1/2,1/2)\)'

4. \(4'^-\)
   \((0,0,1/2)\)
   \((0,1/2,z)\)
   \((4z^{-1},3/2,1/2,1/2)\)'

5. \(\bar{T}'\)
   \((3/4,1/4,1/2)\)
   \((1/2,1/2,1/2)\)'

6. \(n'\)
   \((3/2,1/2,0)\)
   \((mz,3/2,1/2,1/2)\)'

7. \(4'^+\)
   \((1/2,1/2,z; 1/2,2,0)\)
   \((4z,1,0,0)\)'

8. \(4'^-\)
   \((1/2,1/2,z; 1/2,2,0)\)
   \((4z^{-1},1,0,0)\)'

---

86.6.732 - 1 - 1456
Generators selected  (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
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<td>x,y,z [u,v,w]</td>
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<td>(3)</td>
<td>y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(8)</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'

a* = (a - b)/2  b* = (a + b)/2

Origin at 0,0,z

Along [1,0,0] p2mg1'

a* = b  b* = c

Origin at x,1/4,1/4

Along [1,1,0] p2m1'm'

a* = -c  b* = (-a + b)/2

Origin at x,x,1/4
Origin at center (4/m)

Asymmetric unit: \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\)

Symmetry Operations

For (0,0,0) + set:

1. \(1\)
   \((1, 0, 0, 0)\)
2. \(2\)
   \((0, 0, z)\)
   \((2z, 0, 0, 0)\)
3. \(4^+\)
   \((0, 0, z)\)
   \((4z, 0, 0, 0)\)
4. \(4^{-}\)
   \((0, 0, z)\)
   \((4z, 0, 0, 0)\)

For (1/2,1/2,1/2) + set:

1. \(t\)
   \((1/2,1/2,1/2)\)
   \((1,1/2,1/2,1/2)\)
2. \(2\)
   \((0,0,1/2)\)
   \(1/4,1/4,z\)
   \((2z,1/2,1/2,1/2)\)
3. \(4^+\)
   \((0,0,1/2)\)
   \(0,1/2,z\)
   \((4z,1/2,1/2,1/2)\)
4. \(4^{-}\)
   \((0,0,1/2)\)
   \(1/2,0,z\)
   \((4z,1/2,1/2,1/2)\)

5. \(1/4,1/4,1/4\)
   \((1/2,1/2,1/2)\)
   \((1/2,1,2,1/2)\)
6. \(n\)
   \((1/2,1/2,0)\)
   \(x,y,1/4\)
   \((mz,1/2,1/2,1/2)\)
7. \(4^+\)
   \(1/2,0,z\)
   \(1/2,0,1/4\)
   \((4z,1/2,1/2,1/2)\)
8. \(4^{-}\)
   \(0,1/2,z\)
   \(0,1/2,1/4\)
   \((4z,1/2,1/2,1/2)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

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<td>(4) x,z [v,u,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<td>y,0 [0,0,w]</td>
</tr>
<tr>
<td>8 g 2..</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
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<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 f 1</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>3/4,1/4,1/4 [v,u,w]</td>
</tr>
<tr>
<td>4 e 4..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 d 4..</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 c 2/m..</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2 b 4/m..</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 4/m..</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p4  Along [1,0,0]  c2'mm'  Along [1,1,0]  p2'mm'
\( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  \( a^* = -c \)  \( b^* = b \)  \( a^* = -c/2 \)  \( b^* = (-a + b)/2 \)
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
**Origin** at center \((4/m1')\)

**Asymmetric unit** \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\)

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

1. \(1\)
2. \(\tilde{1}\)
3. \(2\)
4. \(4^+\)

For \((1/2,1/2,1/2) + \text{ set}\)

5. \(1\)
6. \(m\)
7. \(4^+\)
8. \(4^+\)
Continued 87.2.734 I4/m1'

For (0,0,0)′ + set

(1) 1′  (1) 0,0,0)′
(2) 2′  0,0,z  (2) 0,0,0)
(3) 4′  0,0,z  (3) 0,0,0)
(4) 4′  0,0,z  (4) 0,0,0)

(5) T′  0,0,0  (5) 0,0,0)
(6) m′  x,y,0  (6) 0,0,0)
(7) 4′  0,0,z; 0,0,0  (7) 0,0,0)
(8) 4′  0,0,z; 0,0,0  (8) 0,0,0)

For (1/2,1,2,1/2)′ + set

(1) t′  (1/2,1/2,1/2)  (1) 1/2,1/2,1/2)
(2) 2′  (0,0,1/2; 1/2,1/2,1/2)′  (2) 1/2,1/2,1/2)
(3) 4′  (0,0,1/2; 1/2,1/2,1/2)′  (3) 1/2,1/2,1/2)
(4) 4′  (0,0,1/2; 1/2,1/2,1/2)′  (4) 1/2,1/2,1/2)

(5) T′  (1/4,1/4,1/4)  (5) 1/2,1/2,1/2)
(6) n′  (1/2,1/2,0)  (6) 1/2,1/2,1/2)
(7) 4′  (1/2,0,1/4; 1/2,0,1/4)  (7) 1/2,1/2,1/2)
(8) 4′  (0,1/2,0; 0,1/2,1/4)  (8) 1/2,1/2,1/2)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1′.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

\[
\begin{array}{cccc}
\text{Coordinates} & \text{Site Symmetry} \\
(0,0,0) + & \text{0,0,0) +} \\
(1/2,1/2,1/2') & \text{(1/2,1/2,1/2') +} \\
\hline
16 & \text{i} & 11' & \text{(1) x,y,z [0,0,0]} \\
(5) & \text{x,} & \text{y,} & \text{z [0,0,0]} \\
8 & \text{h} & \text{m}.1' & \text{x,y,0 [0,0,0]} \\
(6) & \text{x,} & \text{y,} & \text{z [0,0,0]} \\
8 & \text{g} & \text{2..1'} & \text{1/2,0,z [0,0,0]} \\
(7) & \text{y,} & \text{x,} & \text{z [0,0,0]} \\
8 & \text{f} & \text{1..1'} & \text{1/4,1/4,1/4 [0,0,0]} \\
(8) & \text{y,} & \text{x,} & \text{z [0,0,0]} \\
4 & \text{e} & \text{4..1'} & \text{0,0,z [0,0,0]} \\
(4) & \text{y,} & \text{x,} & \text{z [0,0,0]} \\
4 & \text{d} & \text{4..1'} & \text{0,1/2,0 [0,0,0]} \\
(1/2,0,1/4 [0,0,0]} \\
4 & \text{c} & \text{2/m..1'} & \text{0,1/2,0 [0,0,0]} \\
(1/2,0,1/4 [0,0,0]} \\
2 & \text{b} & \text{4/m..1'} & \text{0,0,1/2 [0,0,0]} \\
2 & \text{a} & \text{4/m..1'} & \text{0,0,0 [0,0,0]} \\
\end{array}
\]

Symmetry of Special Projections

Along [0,0,1] p41′
\[a^* = \frac{(a - b)}{2}, \quad b^* = \frac{(a + b)}{2}\]
Origin at 0,0,z

Along [1,0,0] c2mm1′
\[a^* = b, \quad b^* = c\]
Origin at x,0,0

Along [1,1,0] p2mm1′
\[a^* = \frac{(-a + b)}{2}, \quad b^* = \frac{c}{2}\]
Origin at x,x,0
**I4'/m 4'/m Tetragonal**

**Origin** at center (4'/m)

**Asymmetric unit**

\[ 0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/4 \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \((1, 0, 0, 0)\)
2. \((2, 0, 0, z)\)
3. \((4^{+}, 0, 0, z)\)
4. \((4^{-}, 0, 0, z)\)
5. \((1/2, 1/2, 1/2)\)
6. \((x, y, 0)\)
7. \((4^{+}, 0, 0, z; 0,0,0)\)
8. \((4^{-}, 0,0,0)\)

For \((1/2,1/2,1/2)\) + set

1. \((1/2,1/2,1/2)\)
2. \((2, 0, 0, 1/2)\)
3. \((4^{+}, 0, 0, 1/2)\)
4. \((4^{-}, 0, 0, 1/2)\)
5. \((1/4,1/4,1/4)\)
6. \((x, y, 1/4)\)
7. \((4^{+}, 1/2,0, z; 1/2,0,1/4)\)
8. \((4^{-}, 1/2,0,1/4)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'  Along [1,0,0] c2mm'  Along [1,1,0] p2mm'
a* = (a - b)/2  b* = (a + b)/2  a* = -c  b* = b  a* = -c/2  b* = (-a + b)/2
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
**Origin** at center (4/m’)

**Asymmetric unit**

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4} \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \(1\)
   \( (1,0,0,0) \)

2. \(2\)
   \( (2,0,0,z) \)
   \( (2z,0,0,0) \)

3. \(4^+\)
   \( (0,0,z) \)
   \( (4z,0,0,0) \)

4. \(4\)
   \( (0,0,z) \)
   \( (4z^{-1},0,0,0) \)

5. \(T_1\)
   \( (0,0,0) \)
   \( (1,0,0,0') \)

6. \(m_1\)
   \( x,y,0 \)
   \( (mz,0,0,0) \)

7. \(4^+\)
   \( (0,0,z) \)
   \( (4z,0,0,0) \)

8. \(4^+\)
   \( (0,0,z) \)
   \( (4z^{-1},0,0,0) \)

For \((1/2,1/2,1/2) + \) set

1. \(t\)
   \( (1/2,1/2,1/2,1/2) \)
   \( (1/2,1/2,1/2,1/2) \)

2. \(2\)
   \( (0,0,1/2) \)
   \( (1/4,1/4,z) \)
   \( (2z,1/2,1/2,1/2) \)

3. \(4^+\)
   \( (0,0,1/2) \)
   \( (1/2,1/2,1/2) \)
   \( (4z,1/2,1/2,1/2) \)

4. \(4^+\)
   \( (0,0,1/2) \)
   \( (1/2,0,0) \)
   \( (4z^{-1},1/2,1/2,1/2) \)

5. \(T_1\)
   \( (1/4,1/4,1/4) \)
   \( (1/2,1/2,1/2) \)

6. \(n'\)
   \( (1/2,1/2,0) \)
   \( x,y,1/4 \)
   \( (mz,1/2,1/2,1/2) \)

7. \(4^+\)
   \( (1/2,0,1/4) \)
   \( (1/2,0,1/4) \)
   \( (4z,1/2,1/2,1/2) \)

8. \(4^+\)
   \( (1/2,0,1/4) \)
   \( (1/2,0,1/4) \)
   \( (4z^{-1},1/2,1/2,1/2) \)
Continued

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
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<tr>
<td>16 i</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 e</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 d</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [1,1,0]</th>
<th>Along [1,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p41′</td>
<td>a′ = (a - b)/2</td>
<td>b′ = (a + b)/2</td>
<td>a′ = b</td>
<td>b′ = c</td>
</tr>
<tr>
<td>c2m′</td>
<td>a′ = b</td>
<td>b′ = c</td>
<td>a′ = (-a + b)/2</td>
<td>b′ = c/2</td>
</tr>
<tr>
<td>p2m′</td>
<td>a′ = (-a + b)/2</td>
<td>b′ = c/2</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

87.4.736 - 2 - 1465
**Origin** at center (4'/m')

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \(1\)
   1
   (1|0,0,0)

2. \(2\)
   2
   0,0,z (2z|0,0,0)

3. \(4^+\)
   4^+
   0,0,z
   (4z|0,0,0)

4. \(4^-\)
   4^-
   0,0,z
   (4z^-1|0,0,0)

5. \(\overline{1}\)
   \(\overline{1}\)
   0,0,0
   (1|0,0,0)

6. \(m\)
   \(m\)
   x,y,0
   (mz|0,0,0)

7. \(4^+\)
   4^+
   0,0,z; 0,0,0
   (4z|0,0,0)

8. \(4^-\)
   4^-
   0,0,z; 0,0,0
   (4z^-1|0,0,0)

For \((1/2,1/2,1/2) + \) set

1. \(t\)
   (1/2,1/2,1/2)

2. \(2\)
   2
   (0,0,1/2) 1/4,1/4,z
   (2z|1/2,1/2,1/2)

3. \(4^+\)
   4^+
   (0,0,1/2) 0,1/2,z
   (4z|1/2,1/2,1/2)

4. \(4^-\)
   4^-
   (0,0,1/2) 1/2,0,z
   (4z^-1|1/2,1/2,1/2)

5. \(\overline{1}\)
   \(\overline{1}\)
   1/4,1/4,1/4
   (1|0,0,0)

6. \(n\)
   \(n\)
   (1/2,1/2,0) x,y,1/4
   (mz|1/2,1/2,1/2)

7. \(4^+\)
   4^+
   1/2,0,z; 1/2,0,1/4
   (4z|1/2,1/2,1/2)

8. \(4^-\)
   4^-
   0,1/2,z; 0,1/2,1/4
   (4z^-1|1/2,1/2,1/2)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 h m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 g 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 f 1/4</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 e 4'..</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 d 4'..</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>1/2,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 c 2/m'..</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b 4/m'..</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 4/m'..</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'  Along [1,0,0] c2m'm'  Along [1,1,0] p2m'm'
\( a^* = -b^*/2 \quad b^* = (a+b)/2 \)

Origin at 0,0,0
**Origin** at center (4/m)

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \(1\)
2. \(2 \quad 0,0,z\)
3. \(4^+ \quad 0,0,z\)
4. \(4^- \quad 0,0,z\)

For \((1/2,1/2,1/2)\) set

5. \(T \quad 0,0,0\)
6. \(m \quad x,y,0\)
7. \(4^+ \quad 0,0,z; 0,0,0\)
8. \(4^- \quad 0,0,0; 0,0,0\)

For \((1/2,1/2,1/2)\)' set

9. \(t' \quad 1/2,1/2,1/2\)
10. \(2' \quad 0,0,1/2\)
11. \(4^+ \quad 0,0,1/2\)
12. \(4^- \quad 0,0,1/2\)

13. \(T' \quad 1/4,1/4,1/4\)
14. \(n' \quad 1/2,1/2,0\)
15. \(4^+ \quad 1/2,0,1/2\)
16. \(4^- \quad 1/2,0,1/2\)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
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<th>Coordinates</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>16 i 1 x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
<tr>
<td>8 h m.. x,y,0 [0,0,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>8 g 2.. 0,1/2,z [0,0,w]</td>
<td>(3) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>8 f 1/4,1/4,1/4 [0,0,0]</td>
<td>(4) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>4 e 4.. 0,0,z [0,0,w]</td>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 d 1/2,1/4 [0,0,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 c 2/m.. 0,1/2,0 [0,0,w]</td>
<td>(7) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 4/m.. 0,0,1/2 [0,0,w]</td>
<td>(8) y,x,z [v,u,w]</td>
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<tr>
<td>2 a 4/m.. 0,0,0 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p..4  Along [1,0,0]  c..2'mm'  Along [1,1,0]  p..2m'm'

\[ a^* = (a - b)/2 \; b^* = (a + b)/2 \]

Origin at 0,0,z

Along [1,0,0]  c..2'mm'

\[ a^* = -c \; b^* = b \]

Origin at x,0,0

Along [1,1,0]  p..2m'm'

\[ a^* = -c/2 \; b^* = (-a + b)/2 \]

Origin at x,x,1/4

87.6.738 - 2 - 1469
Origin at center (4'/m)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2_1 | 0,0,0)

(5) m 0,0,0
(1 | 0,0,0)

(6) m x,y,0
(m_1 | 0,0,0)

(3) 4^+ 0,0,z
(4_1 | 0,0,0)'

(4) 4^- 0,0,z
(4_1^- | 0,0,0)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)'

(2) 2' (0,0,1/2) 1/4,1/4,z
(2_2 | 1/2,1/2,1/2)'

(5) n' (1/2,1/2,0) x,y,1/4
(m_2 | 1/2,1/2,1/2)'

(6) n' (1/2,1/2,0) x,y,1/4
(m_2 | 1/2,1/2,1/2)'

(3) 4^+ (0,0,1/2) 0,1/2,z
(4_2 | 1/2,1/2,1/2)

(4) 4^- (0,0,1/2) 1/2,0,z
(4_2^- | 1/2,1/2,1/2)

(7) 4^+ 1/2,0,z; 1/2,0,1/4
(4_2 | 1/2,1/2,1/2)

(8) 4^- 0,1/2,z; 0,1/2,1/4
(4_2^- | 1/2,1/2,1/2)
**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16</th>
<th>i</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) ( \bar{x},\bar{y},z [u,v,w] )</th>
<th>(3) ( y,x,z [v,u,w] )</th>
<th>(4) ( y,\bar{x},z [v,u,w] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>h</td>
<td>1</td>
<td>x,y,0 [0,0,w]</td>
<td>( \bar{x},\bar{y},0 [0,0,w] )</td>
<td>( y,x,0 [0,0,w] )</td>
<td>( y,\bar{x},0 [0,0,w] )</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
<td>2</td>
<td>0,1/2,2 [0,0,w]</td>
<td>1/2,0,2 [0,0,w]</td>
<td>0,1/2,( \bar{z} [0,0,w] )</td>
<td>1/2,0,( \bar{z} [0,0,w] )</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>1</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,1/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>4</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,( \bar{z} [0,0,0] )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>4</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>2</td>
<td>0,1/2,2 [0,0,w]</td>
<td>1/2,0,2 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] ( p_\sigma 4 )</th>
<th>Along [1,0,0] ( c_\sigma 2'an )</th>
<th>Along [1,1,0] ( p_{2\alpha} 2'm'm' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = (a-b)/2 ) ( b^* = (a+b)/2 )</td>
<td>( a^* = -c ) ( b^* = b )</td>
<td>( a^* = -c/2 ) ( b^* = (-a+b)/2 )</td>
</tr>
<tr>
<td>Origin at 1/2,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,1/4</td>
</tr>
</tbody>
</table>
Origin at center (4/m')

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(5) 1/2,1/2,1/2' + set

(1) t' (1/2,1/2,1/2)
(1/2,1/2,1/2')

(6) n (1/2,1/2,0)
(1/2,1/2,1/2)

(4) 4' 0,0,0
(4 | 0,0,0)

(4) 4' 0,0,0
(4 | 0,0,0)

(4) 4' 0,0,0
(4 | 0,0,0)

(5) 1/2,1/2,1/2' + set

(1) t' (1/2,1/2,1/2)
(1/2,1/2,1/2')

(6) n (1/2,1/2,0)
(1/2,1/2,1/2)

(4) 4' 1/2,0,0
(4 | 1/2,1/2,1/2)

(4) 4' 1/2,0,0
(4 | 1/2,1/2,1/2)

(4) 4' 1/2,0,0
(4 | 1/2,1/2,1/2)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 i 1</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>16 i 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 i 1</td>
<td>(1/2,1/2,1/2)</td>
</tr>
<tr>
<td>16 i 1</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>16 i 1</td>
<td>(v,u,w)</td>
</tr>
</tbody>
</table>

| 8 h m'..     | x,y,0 [u,v,0] |
| 8 h m'..     | x,y,0 [u,v,0] |
| 8 h m'..     | y,x,0 [v,u,0] |
| 8 h m'..     | y,x,0 [v,u,0] |
| 8 g 2..      | 0,1/2,z [0,0,w] |
| 8 g 2..      | 1/2,0,z [0,0,w] |
| 8 g 2..      | 0,1/2,z [0,0,w] |
| 8 g 2..      | 1/2,0,z [0,0,w] |
| 8 f 1        | 1/4,1/4,1/4 [u,v,w] |
| 8 f 1        | 3/4,3/4,1/4 [u,v,w] |
| 8 f 1        | 3/4,1/4,1/4 [v,u,w] |
| 8 f 1        | 1/4,3/4,1/4 [v,u,w] |
| 4 e 4..      | 0,0,z [0,0,w] |
| 4 e 4..      | 0,0,z [0,0,w] |
| 4 e 4..      | 0,0,z [0,0,w] |
| 4 d 4'..     | 0,1/2,1/4 [0,0,0] |
| 4 d 4'..     | 1/2,0,1/4 [0,0,0] |
| 4 c 2/m'..   | 0,1/2,0 [0,0,0] |
| 4 c 2/m'..   | 1/2,0,0 [0,0,0] |
| 2 b 4/m'..   | 0,0,1/2 [0,0,0] |
| 2 b 4/m'..   | 0,0,0 [0,0,0] |
| 2 a 4/m'..   | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1]  
**a** = (a - b)/2  
**b** = (a + b)/2  
Origin at 0,0,z

Along [1,0,0]  
**c** = 2m'm'  
**a** = b  
**b** = c  
Origin at x,0,0

Along [1,1,0]  
**p** = 2m'm'  
**a** = -c/2  
**b** = (-a + b)/2  
Origin at x,x,0
**Origin** at center (4'/m')

**Asymmetric unit**

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4
\]

**Symmetry Operations**

For \((0,0,0)\) + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1))</td>
<td>((0,0,0))</td>
</tr>
<tr>
<td>((2))</td>
<td>((0,0,z))</td>
</tr>
<tr>
<td>((3))</td>
<td>((0,0,z))</td>
</tr>
<tr>
<td>((4))</td>
<td>((0,0,z))</td>
</tr>
<tr>
<td>((5))</td>
<td>((0,0,0))</td>
</tr>
<tr>
<td>((6))</td>
<td>((x,y,0))</td>
</tr>
<tr>
<td>((7))</td>
<td>((0,0,z))</td>
</tr>
<tr>
<td>((8))</td>
<td>((0,0,z))</td>
</tr>
</tbody>
</table>

For \((1/2,1/2,1/2)\) + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1))</td>
<td>((1/2,1/2,1/2))</td>
</tr>
<tr>
<td>((2))</td>
<td>((0,0,1/2))</td>
</tr>
<tr>
<td>((3))</td>
<td>((0,0,1/2))</td>
</tr>
<tr>
<td>((4))</td>
<td>((0,0,1/2))</td>
</tr>
<tr>
<td>((5))</td>
<td>((1/4,1/4,1/4))</td>
</tr>
<tr>
<td>((6))</td>
<td>((1/2,1/2,0))</td>
</tr>
<tr>
<td>((7))</td>
<td>((1/2,0,1/2))</td>
</tr>
<tr>
<td>((8))</td>
<td>((0,1/2,0))</td>
</tr>
</tbody>
</table>
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2)'+</td>
</tr>
<tr>
<td>16 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(3) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(4) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(6) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(8) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>8 h m'..</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>(9) x,y,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>(10) y,x,0 [v,u,0]</td>
<td></td>
</tr>
<tr>
<td>(11) y,x,0 [v,u,0]</td>
<td></td>
</tr>
<tr>
<td>8 g 2..</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>1/2,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>0,1/2,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>1/2,0,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>8 f 1</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
</tr>
<tr>
<td>3/4,3/4,1/4 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>3/4,1/4,1/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>3/4,3/4,1/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>4 e 4'..</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>0,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 d 4'..</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td>1/2,0,1/4 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 c 2/m'..</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>1/2,0,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 4'/m'..</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 4'/m'..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p41'  Along [1,0,0] c₉ 2m'm'  Along [1,1,0] p₂a 2m'm'

\[ a^* = (a - b)/2 \]
\[ b^* = (a + b)/2 \]

Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
I4₁/a  
 origin at -4 at 0,-1/4,-1/8 from 1  
 asymmetric unit 0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1  
 symmetry operations  
 for (0,0,0) set  
 (1) 1  
 (2) 2 0,0,z  
 (3) 4⁺ (0,0,1/4) -1/4,1/4,z  
 (4) 4⁻ (0,0,1/4) 1/4,1/4,z  
 (5) 1/4,0,1/8  
 (6) b (0,1/2,0) x,y,1/8  
 (7) 4⁺ 0,0,z; 0,0,0  
 (8) 4⁻ 0,0,z; 0,0,0  
 for (1/2,1/2,1/2) set  
 (1) 1  
 (2) 2 (0,0,1/2) 1/4,1/4,z  
 (3) 4⁺ (0,0,3/4) 1/4,1/4,z  
 (4) 4⁻ (0,0,3/4) 1/4,-1/4,z  
 (5) 1/4,0,3/8  
 (6) a (1/2,0,0) x,y,3/8  
 (7) 4⁺ 1/2,0,z; 1/2,0,1/4  
 (8) 4⁻ 0,1/2,z; 0,1/2,1/4  
 88.1.742 - 1 - 1476
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tr>
<td>16 f</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>(5) x,y+1/2,z+1/4 [u,v,w]</td>
<td>(6) x,y+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
</tbody>
</table>

| 8 e 2 | 0,0,z [0,0,w] | 0,0,z [0,0,w] | 0,1/2,z+1/4 [0,0,w] | 0,1/2,z+1/4 [0,0,w] |
| 8 d 1 | 0,1/4,5/8 [u,v,w] | 0,3/4,5/8 [u,v,w] | 1/4,0,3/8 [u,v,w] | 3/4,0,3/8 [u,v,w] |
| 8 c 1 | 0,1/4,1/8 [u,v,w] | 0,3/4,1/8 [u,v,w] | 1/4,0,7/8 [u,v,w] | 3/4,0,7/8 [u,v,w] |
| 4 b 4.. | 0,0,1/2 [0,0,w] | 0,1/2,3/4 [0,0,w] |             |             |
| 4 a 4.. | 0,0,0 [0,0,w] | 0,1/2,1/4 [0,0,w] |             |             |

Symmetry of Special Projections

Along [0,0,1] p4  
\[ a^* = a / 2 \quad b^* = b / 2 \]
Origin at 0,0,z

Along [1,0,0] c2' mm'  
\[ a^* = -c \quad b^* = b \]
Origin at x,0,3/8

Along [1,1,0] p2'm'g  
\[ a^* = (a + b) / 2 \quad b^* = c / 2 \]
Origin at x,x+1/4,1/8
I4₁/a₁′

88.2.743

Tetragonal

Origin at 1' at 0,-1/4,-1/8 from 1 1'

Asymmetric unit
0 ≤ x ≤ 1/4; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1

Symmetry Operations

For (0,0,0) + set

| (1) 1 (1 | 0,0,0) |
| (2) 2 0,0,z (2z | 0,0,0) |
| (3) 4* (0,0,1/4) -1/4,1/4,z (4z | 0,1/2,1/4) |
| (4) 4' (0,0,1/4) 1/4,1/4,z (4z⁻¹ | 0,1/2,1/4) |

(5) 0,1/4,1/8 (1 | 0,1/2,1/4)

(6) b (0,1/2,0) x,y,1/8 (mz | 0,1/2,1/4)

(7) 4* 0,0,z; 0,0,0 (4z | 0,0,0)

(8) 4' 0,0,z; 0,0,0 (4z⁻¹ | 0,0,0)

For (1/2,1/2,1/2) + set

| (1) t (1/2,1/2,1/2) (1 | 1/2,1/2,1/2) |
| (2) 2 (0,0,1/2) 1/4,1/4,z (2z | 1/2,1/2,1/2) |
| (3) 4* (0,0,3/4) 1/4,1/4,z (4z | 1/2,0,3/4) |
| (4) 4' (0,0,3/4) 1/4,1/4,z (4z⁻¹ | 1/2,0,3/4) |

(5) 1/4,0,3/8 (1 | 1/2,0,3/4)

(6) a (1/2,0,0) x,y,3/8 (mz | 1/2,0,3/4)

(7) 4* 1/2,0,z; 1/2,0,1/4 (4z | 1/2,1/2,1/2)

(8) 4' 0,1/2,z; 0,1/2,1/4 (4z⁻¹ | 1/2,1/2,1/2)
Continued

For \((0,0,0)\)' + set

\begin{align*}
(1) & \quad \text{1'}\, (0,0,0)' \\
(2) & \quad 2'\, 0,0,z \\
(3) & \quad 4'^+ (0,0,1/4) -1/4,1/4,z \\
(4) & \quad 4'\, (0,0,1/4) 1/4,1/4,z \quad (4_z' 0,1/2,1/4)' \\
(5) & \quad 1', 0,1/4,1/8 \\
& \quad (1, 0,1/4,1/8)' \\
& \quad (2, 0,1/4,1/8)' \\
& \quad (3, 0,1/4,1/8)' \\
& \quad (4, 0,1/4,1/8)' \\
(6) & \quad b' (0,1/2,0) \quad x,y,1/8 \\
& \quad (m_z, 0,1/2,1/4)' \\
(7) & \quad 4'^- 0,0,z; 0,0,0 \\
& \quad (4_z, 0,0,0)' \\
(8) & \quad 4^- 0,0,z; 0,0,0 \\
& \quad (4_z, 0,0,0)' \\
(1) & \quad t' (1/2,1/2,1/2) \\
& \quad (1, 1/2,1/2,1/2)' \\
(2) & \quad 2' (0,0,1/2) \quad 1/4,1/4,z \\
& \quad (2, 1/2,1/2,1/2)' \\
(3) & \quad 4'^+ (0,0,3/4) 1/4,1/4,z \\
& \quad (4_z, 1/2,0,3/4)' \\
(4) & \quad 4'\, (0,0,3/4) 1/4,-1/4,z \\
& \quad (4_z, 1/2,0,3/4)' \\
(5) & \quad 1'/4,0,3/8 \\
& \quad (1, 1/2,0,3/4)' \\
& \quad (2, 1/2,0,3/4)' \\
& \quad (3, 1/2,0,3/4)' \\
& \quad (4, 1/2,0,3/4)' \\
(6) & \quad a' (1/2,0,0) \quad x,y,3/8 \\
& \quad (m_z, 1/2,0,3/4)' \\
(7) & \quad 4'^+ 1/2,0,z; 1/2,0,1/4 \\
& \quad (4_z, 1/2,1/2,1/2)' \\
(8) & \quad 4^- 0,1/2,z; 0,1/2,1/4 \\
& \quad (4_z, 1/2,1/2,1/2)' \\
\end{align*}

Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'. \)

Positions

\begin{tabular}{llll}
\textbf{Multiplicity} & \textbf{Wyckoff letter} & \textbf{Site Symmetry} \\
16 & f & 11' & (1) x,y,z [0,0,0] \\
 & & & (2) x,y,z [0,0,0] \\
 & & & (3) y,x+1/2,z+1/4 [0,0,0] \\
 & & & (4) y,x+1/2,z+1/4 [0,0,0] \\
 & & & (5) x,y+1/2,z+1/4 [0,0,0] \\
 & & & (6) x,y+1/2,z+1/4 [0,0,0] \\
 & & & (7) y,x,z [0,0,0] \\
 & & & (8) y,x,z [0,0,0] \\
8 & e & 21' & 0,0,z [0,0,0] \\
 & & & 0,0,z [0,0,0] \\
 & & & 0,1/2,z+1/4 [0,0,0] \\
 & & & 0,1/2,z+1/4 [0,0,0] \\
8 & d & 11' & 0,1/4,5/8 [0,0,0] \\
 & & & 0,3/4,5/8 [0,0,0] \\
 & & & 1/4,0,3/8 [0,0,0] \\
 & & & 3/4,0,3/8 [0,0,0] \\
8 & c & 11' & 0,1/4,1/8 [0,0,0] \\
 & & & 0,3/4,1/8 [0,0,0] \\
 & & & 1/4,0,7/8 [0,0,0] \\
 & & & 3/4,0,7/8 [0,0,0] \\
4 & b & 4..1' & 0,0,1/2 [0,0,0] \\
 & & & 0,1/2,3/4 [0,0,0] \\
4 & a & 4..1' & 0,0,0 [0,0,0] \\
 & & & 0,1/2,1/4 [0,0,0] \\
\end{tabular}

Symmetry of Special Projections

\begin{align*}
\text{Along } [0,0,1] & \quad \text{p41}^* \\
\text{Along } [1,0,0] & \quad \text{c2mm}^1 \\
\text{Along } [1,1,0] & \quad \text{p2mg}^1 \\
\text{Origin at } 0,0,z & \quad \text{Origin at } x,0,3/8 \\
\text{Origin at } x+1/4,1/8 & \quad \text{Origin at } x, x+1/4,1/8 \\
\end{align*
Origin at $\bar{4}$ at $0,-1/4,-1/8$ from $\bar{1}$

Asymmetric unit  
$0 \leq x < 1/4$;  
$0 \leq y < 1/4$;  
$0 \leq z < 1$

Symmetry Operations

For $(0,0,0) + \text{ set}$

(1) $1$
$1 \ 0,0,0$  
(2) $2 \ 0,0,z$  
$2_z \ 0,0,0$  
(3) $4^{+}\ (0,0,1/4) \ -1/4,1/4,z$  
$4_z \ 0,1/2,1/4'$  
(4) $4^{-}\ (0,0,1/4) \ 1/4,1/4,z$  
$4_{z^{-1}} \ 0,1/2,1/4'$

(5) $\bar{1} \ 0,1/4,1/8$  
$1 \ 0,1/2,1/4$  
(6) $b \ (0,1/2,0) \ x,y,1/8$  
$m_z \ 0,1/2,1/4$  
(7) $\bar{4}^{+}\ 0,0,z; 0,0,0$  
$4_z \ 0,0,0'$  
(8) $\bar{4}^{-}\ 0,0,z; 0,0,0$  
$4_{z^{-1}} \ 0,0,0'$

For $(1/2,1/2,1/2) + \text{ set}$

(1) $t \ (1/2,1/2,1/2)$  
$1 \ 1/2,1/2,1/2$  
(2) $2 \ (0,0,1/2) \ 1/4,1/4,z$  
$2_z \ 1/2,1/2,1/2$  
(3) $4^{+}\ (0,0,3/4) \ 1/4,1/4,z$  
$4_z \ 1/2,0,3/4'$  
(4) $4^{-}\ (0,0,3/4) \ 1/4,-1/4,z$  
$4_{z^{-1}} \ 1/2,0,3/4'$

(5) $\bar{1} \ 1/4,0,3/8$  
$1 \ 1/2,0,3/4$  
(6) $a \ (1/2,0,0) \ x,y,3/8$  
$m_z \ 1/2,0,3/4$  
(7) $\bar{4}^{+}\ 1/2,0,z; 1/2,0,1/4$  
$4_z \ 1/2,1/2,1/2'$  
(8) $\bar{4}^{-}\ 0,1/2,z; 0,1/2,1/4$  
$4_{z^{-1}} \ 1/2,1/2,1/2'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>16 f</td>
<td>1 (1) x,y,z [u,v,w]</td>
<td></td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(3) x,y+1/2,z+1/4 [v,u,w]</td>
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<tr>
<td></td>
<td></td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
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<td></td>
<td>(5) x,y+1/2,z+1/4 [u,v,w]</td>
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<tr>
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<td></td>
<td>(6) y,x+1/2,z+1/4 [v,u,w]</td>
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<td></td>
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<td>(7) y,x,z [v,u,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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<td></td>
</tr>
<tr>
<td>8 e</td>
<td>2</td>
<td>0,0,z [0,0,w]</td>
<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,z+1/4 [0,0,w]</td>
<td></td>
<td>0,1/2,z+1/4 [0,0,w]</td>
</tr>
<tr>
<td>8 d</td>
<td>1</td>
<td>0,1/4,5/8 [u,v,w]</td>
<td></td>
<td>0,3/4,5/8 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/4,0,3/8 [v,u,w]</td>
<td></td>
<td>3/4,0,3/8 [v,u,w]</td>
</tr>
<tr>
<td>8 c</td>
<td>1</td>
<td>0,1/4,1/8 [u,v,w]</td>
<td></td>
<td>0,3/4,1/8 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/4,0,7/8 [v,u,w]</td>
<td></td>
<td>3/4,0,7/8 [v,u,w]</td>
</tr>
<tr>
<td>4 b</td>
<td>4'..</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,1/4 [0,0,0]</td>
<td></td>
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</tr>
<tr>
<td>4 a</td>
<td>4'..</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'  
Along [1,0,0] c2'mm'  
Along [1,1,0] p2'm'g

\(a^* = a/2 \quad b^* = b/2\)  
\(a^* = -c \quad b^* = b\)  
\(a^* = -(a+b)/2 \quad b^* = c/2\)

Origin at 0,0,z  
Origin at x,0,3/8  
Origin at x,x+1/4,1/8
**Symmetry Operations**

For $(0,0,0)$ set:

1. $I \cdot 0,0,0$
2. $2 \cdot 0,0,z$
3. $4^+ \cdot (0,0,1/4) \cdot -1/4,1/4,z$
4. $4^- \cdot (0,0,1/4) \cdot 1/4,1/4,z$
5. $I \cdot 1/4,0,3/8$
6. $b' \cdot (0,1/2,0) \cdot x,y,1/8$
7. $4^+ \cdot 0,0,z \cdot 0,0,0$
8. $4^- \cdot 0,0,z \cdot 0,0,0$

For $(1/2,1/2,1/2)$ set:

1. $t \cdot (1/2,1/2,1/2)$
2. $2 \cdot (0,0,1/2) \cdot 1/4,1/4,z$
3. $4^+ \cdot (0,0,3/4) \cdot 1/4,1/4,z$
4. $4^- \cdot (0,0,3/4) \cdot 1/4,1/4,z$
5. $T \cdot 1/4,0,3/8$
6. $a' \cdot (1/2,0,0) \cdot x,y,3/8$
7. $4^+ \cdot 1/2,0,z \cdot 1/2,0,1/4$
8. $4^- \cdot 1/2,0,z \cdot 1/2,0,1/4$
**Generators selected**  \( (1) \); \( t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f 1</td>
<td>((1) x,y,z [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>((2) \bar{x},\bar{y},z [\bar{u},\bar{v},w] )</td>
</tr>
<tr>
<td></td>
<td>((3) y,x+1/2,z+1/4 [\bar{v},u,w] )</td>
</tr>
<tr>
<td></td>
<td>((4) \bar{y},x+1/2,z+1/4 [v,\bar{u},w] )</td>
</tr>
<tr>
<td></td>
<td>((5) x,y+1/2,\bar{z}+1/4 [u,v,\bar{w}] )</td>
</tr>
<tr>
<td></td>
<td>((6) y,\bar{x},\bar{z} [v,\bar{u},\bar{w}] )</td>
</tr>
<tr>
<td></td>
<td>((7) y,\bar{x},\bar{z} [v,\bar{u},\bar{w}] )</td>
</tr>
<tr>
<td></td>
<td>((8) \bar{y},x,z [v,u,w] )</td>
</tr>
<tr>
<td>8 e 2</td>
<td>((0,0,0) + (1/2,1/2,1/2) + (0,0,z [0,0,w] 0,0,\bar{z} [0,0,\bar{w}] 0,1/2,z+1/4 [0,0,w] 0,1/2,\bar{z}+1/4 [0,0,\bar{w}] )</td>
</tr>
<tr>
<td>8 d ( \bar{1} )</td>
<td>((0,1/4,5/8 [0,0,0] 0,3/4,5/8 [0,0,0] 1/4,0,3/8 [0,0,0] 3/4,0,3/8 [0,0,0] )</td>
</tr>
<tr>
<td>8 c ( \bar{1} )</td>
<td>((0,1/4,1/8 [0,0,0] 0,3/4,1/8 [0,0,0] 1/4,0,7/8 [0,0,0] 3/4,0,7/8 [0,0,0] )</td>
</tr>
<tr>
<td>4 b ( \bar{4} )</td>
<td>((0,0,1/2 [0,0,0] 0,1/2,3/4 [0,0,0] )</td>
</tr>
<tr>
<td>4 a ( \bar{4} )</td>
<td>((0,0,0 [0,0,0] 0,1/2,1/4 [0,0,0] )</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1] \) p4 \( \text{Along} [1,0,0] \) c2m'm' \( \text{Along} [1,1,0] \) p2m'g' 
  - \( a^* = a/2 \) \( b^* = b/2 \) \( a^* = b \) \( b^* = c \) \( a^* = (-a + b)/2 \) \( b^* = c/2 \)
- Origin at \(1/2,-1/2,z\) \(\text{Origin at } x,0,3/8\) \(\text{Origin at } x,x+1/4,1/8\)
Origin at \( \bar{4} \) at -1/4,-1/8 from \( \bar{1} \).

Asymmetric unit \( 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1 \)

Symmetry Operations

For \((0,0,0) + \) set

\begin{align*}
(1) \quad & \mathbf{1} \\
(1) & (0,0,0) \\
(5) \quad & \bar{1} (0,1/4,1/8) \\
(5) & (1 \mid 0,1/2,1/4)' \\
(6) \quad & \mathbf{b}' (0,1/2,0) x,y,1/8 \\
(6) & (m_x,0,1/2,1/4)' \\
(7) \quad & \mathbf{4}^+ (0,0,0) z; 0,0,0 \\
(7) & (4_z,0,0,0) \\
(8) \quad & \mathbf{4}^- (0,0,0) z; 0,0,0 \\
(8) & (4_z^-|0,0,0) \\
\end{align*}

For \((1/2,1/2,1/2) + \) set

\begin{align*}
(1) \quad & t (1/2,1/2,1/2) \\
(1) & (1/2,1/2,1/2) \\
(5) \quad & \bar{1} (1/4,0,3/8) \\
(5) & (1/2,0,3/4)' \\
(6) \quad & a'(1/2,0,0) x,y,3/8 \\
(6) & (m_x,1/2,0,3/4)' \\
(7) \quad & \mathbf{4}^- (1/2,0,0) z; 1/2,0,1/4 \\
(7) & (4_z^-|1/2,1/2,1/2) \\
(8) \quad & \mathbf{4}^- (0,1/2,0) z; 0,1/2,1/4 \\
(8) & (4_z^-|1/2,1/2,1/2) \\
\end{align*}
Continued

88.5.746

I4, 'l,a'

**Generators selected**  
(1); \(t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).**

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 f</td>
<td>(1) (x, y, z [u, v, w])</td>
</tr>
<tr>
<td></td>
<td>(3) (\bar{y}, x+1/2, z+1/4 [v, u, w])</td>
</tr>
<tr>
<td></td>
<td>(5) (x, \bar{y}+1/2, \bar{z}+1/4 [u, \bar{v}, \bar{w}])</td>
</tr>
<tr>
<td></td>
<td>(7) (y, x, \bar{z} [v, u, w])</td>
</tr>
</tbody>
</table>

| 8 e 2       | 0,0,z [0,0,w] | 0,0,z [0,0,w] | 0,1/2,z+1/4 [0,0,\(w\)] | 0,1/2,z+1/4 [0,0,\(w\)] | 1/4,0,3/8 [0,0,0] | 3/4,0,3/8 [0,0,0] |
| 8 d \(\bar{1}\) | 0,1/4,5/8 [0,0,0] | 0,3/4,5/8 [0,0,0] | 1/4,0,3/8 [0,0,0] | 3/4,0,3/8 [0,0,0] |
| 8 c \(\bar{1}\) | 0,1/4,1/8 [0,0,0] | 0,3/4,1/8 [0,0,0] | 1/4,0,7/8 [0,0,0] | 3/4,0,7/8 [0,0,0] |
| 4 b \(\bar{4}\) | 0,0,1/2 [0,0,w] | 0,1/2,3/4 [0,0,w] |
| 4 a \(\bar{4}\) | 0,0,0 [0,0,w] | 0,1/2,1/4 [0,0,w] |

**Symmetry of Special Projections**

- Along [0,0,1] \(p_2\).4
  - \(a^* = a / 2\) \(b^* = b / 2\)

- Along [1,0,0] \(c2m'\)m'
  - \(a^* = b\) \(b^* = c\)

- Along [1,1,0] \(p2m'\)g'
  - \(a^* = (-a + b) / 2\) \(b^* = c / 2\)

Origin at 0,0,z  
Origin at x,0,3/8  
Origin at x,x+1/4,1/8
**Origin** on 422

**Asymmetric unit** \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \)

**Symmetry Operations**

1. \( 1 \)
   \[ (1|0,0,0) \]

2. \( 2 \)
   \[ (2|0,0,z) \]
   \[ (2_z|0,0,0) \]

3. \( 4^+ \)
   \[ (4|0,0,z) \]
   \[ (4_z|0,0,0) \]

4. \( 4^- \)
   \[ (4|0,0,z) \]
   \[ (4_z^{-1}|0,0,0) \]

5. \( 2 \)
   \[ (5|0,y,0) \]
   \[ (2_y|0,0,0) \]

6. \( 2 \)
   \[ (6|x,0,0) \]
   \[ (2_x|0,0,0) \]

7. \( 2 \)
   \[ (7|x,x,0) \]
   \[ (2_x|x,0) \]

8. \( 2 \)
   \[ (8|x,x,0) \]
   \[ (2_x|x,0) \]

---

**89.1.747**

**P422**

**422**

**Tetragonal**
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td>4 o .2.</td>
<td>x,1/2,0 [u,0,0]</td>
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<tr>
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<td>x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
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<td>4 m .2.</td>
<td>x,1/2,1/2 [u,0,0]</td>
<td>1/2,x,1/2 [0,u,0]</td>
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<tr>
<td>4 l .2.</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
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<td>x,x,1/2 [u,u,0]</td>
<td>x,x,1/2 [u,u,0]</td>
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<tr>
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<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 h 4..</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 g 4..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 f 222.</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2 e 222.</td>
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<tr>
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<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

- **Along [0,0,1]**  p4m'm'
  - a* = a  b* = b
  - Origin at 0,0,z

- **Along [1,0,0]**  p2mm'
  - a* = -c  b* = b
  - Origin at x,0,0

- **Along [1,1,0]**  p2m'm'
  - a* = (-a + b)/2  b* = c
  - Origin at x,x,0
Origin on 4221'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For 1 + set

\[(1) \begin{array}{c} 1 \\ (1,0,0,0) \end{array}
\]

\[(2) \begin{array}{c} 2 \quad 0,0,z \\ (2z,0,0,0) \end{array}
\]

\[(3) \begin{array}{c} 4^+ \quad 0,0,z \\ (4z,0,0,0) \end{array}
\]

\[(4) \begin{array}{c} 4^- \quad 0,0,z \\ (4z^{-1},0,0,0) \end{array}
\]

\[(5) \begin{array}{c} 2 \quad 0,y,0 \\ (2z,0,0,0) \end{array}
\]

\[(6) \begin{array}{c} 2 \quad x,0,0 \\ (2z,0,0,0) \end{array}
\]

\[(7) \begin{array}{c} 2 \quad x,x,0 \\ (2z_y,0,0,0) \end{array}
\]

\[(8) \begin{array}{c} 2 \quad x,x,0 \\ (2z_y,0,0,0)' \end{array}
\]

For 1' + set

\[(1') \begin{array}{c} 1' \\ (1,0,0,0)' \end{array}
\]

\[(2') \begin{array}{c} 2' \quad 0,0,z \\ (2z,0,0,0)' \end{array}
\]

\[(3') \begin{array}{c} 4^+ \quad 0,0,z \\ (4z,0,0,0)' \end{array}
\]

\[(4') \begin{array}{c} 4^- \quad 0,0,z \\ (4z^{-1},0,0,0)' \end{array}
\]

\[(5') \begin{array}{c} 2' \quad 0,y,0 \\ (2z,0,0,0)' \end{array}
\]

\[(6') \begin{array}{c} 2' \quad x,0,0 \\ (2z,0,0,0)' \end{array}
\]

\[(7') \begin{array}{c} 2' \quad x,x,0 \\ (2z_y,0,0,0)' \end{array}
\]

\[(8') \begin{array}{c} 2' \quad x,x,0 \\ (2z_y,0,0,0)' \end{array}
\]
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 +</td>
<td></td>
<td></td>
<td>x,y,z [0,0,0]</td>
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<tr>
<td>1' +</td>
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<td>(7) y,x,z [0,0,0]</td>
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<td>(8) y,x,z [0,0,0]</td>
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<td>0,x,0 [0,0,0]</td>
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<td>x,x,1/2 [0,0,0]</td>
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<td>4 j</td>
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<td>4..1'</td>
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<td>1/2,1/2,z [0,0,0]</td>
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<td></td>
<td>1/2,1/2,z [0,0,0]</td>
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<tr>
<td>2 g</td>
<td>4..1'</td>
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<td>0,0,z [0,0,0]</td>
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<td>222.1'</td>
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<td>0,1/2,1/2 [0,0,0]</td>
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<td>2 e</td>
<td>222.1'</td>
<td></td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
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<td></td>
<td></td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1 d</td>
<td>4221'</td>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
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<td>1 c</td>
<td>4221'</td>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b</td>
<td>4221'</td>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
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<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>1 a</td>
<td>4221'</td>
<td></td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p4mm1'  Along [1,0,0]  p2mm1'  Along [1,1,0]  p2mm1'

a* = a  b* = b  a* = b  b* = c  a* = (-a + b)/2  b* = c

Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
Origin on 4\'22'

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 \(0,0,z\)
\((2_z | 0,0,0)\)

(3) \(4'\) \(0,0,z\)
\((4_z | 0,0,0)'\)

(4) \(4'\) \(0,0,z\)
\((4_z^{-1} | 0,0,0)'\)

(5) 2 \(0,y,0\)
\((2_y | 0,0,0)\)

(6) 2 \(x,0,0\)
\((2_x | 0,0,0)\)

(7) \(2'\) \(x,x,0\)
\((2_{xy} | 0,0,0)'\)

(8) \(2'\) \(x,x,0\)
\((2_{xy} | 0,0,0)'\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 p 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1)</td>
</tr>
<tr>
<td>5</td>
<td>x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 o .2.</td>
<td>x,1/2,0 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 n .2.</td>
<td>x,0,1/2 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 m .2.</td>
<td>x,1/2,1/2 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 l .2.</td>
<td>x,0,0 [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 k ..2'</td>
<td>x,x,1/2 [u,u,w]</td>
<td></td>
</tr>
<tr>
<td>4 j ..2'</td>
<td>x,x,0 [u,u,w]</td>
<td></td>
</tr>
<tr>
<td>4 i 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 h 4'..</td>
<td>1/2,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 g 4'..</td>
<td>0,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 f 222.</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 e 222.</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 d 4'2'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 c 4'2'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 b 4'2'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a 4'2'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Origin at x,0,0</th>
<th>Origin at x,x,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>a* = b</td>
<td>a* = -c</td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = c</td>
<td>b* = (-a + b)/2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on 42'2'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

1. \( 1 \)
   \[ (1|0,0,0) \]
2. \( 2 \)
   \[ 0,0,z \]
   \[ (2_z|0,0,0) \]
3. \( 4' \)
   \[ 0,0,z \]
   \[ (4_z|0,0,0) \]
4. \( 4' \)
   \[ 0,0,z \]
   \[ (4_z^{-1}|0,0,0) \]
5. \( 2' \)
   \[ 0,y,0 \]
   \[ (2_y|0,0,0) \]
6. \( 2' \)
   \[ x,0,0 \]
   \[ (2_x|0,0,0) \]
7. \( 2' \)
   \[ x,x,0 \]
   \[ (2_{xy}|0,0,0) \]
8. \( 2' \)
   \[ x,x,0 \]
   \[ (2_{xy}|0,0,0) \]

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Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Position</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 p 1 (1)</td>
<td>x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 o .2'</td>
<td>x,1/2,0 [u,0,w]</td>
<td>x,1/2,0 [u,0,w]</td>
<td>1/2,x,0 [0,u,w]</td>
</tr>
<tr>
<td>4 n .2'</td>
<td>x,0,1/2 [u,0,w]</td>
<td>x,0,1/2 [u,0,w]</td>
<td>0,x,1/2 [0,u,w]</td>
</tr>
<tr>
<td>4 m .2'</td>
<td>x,1/2,1/2 [u,0,w]</td>
<td>x,1/2,1/2 [u,0,w]</td>
<td>1/2,x,1/2 [0,u,w]</td>
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<tr>
<td>4 l .2'</td>
<td>x,0,0 [u,0,w]</td>
<td>x,0,0 [u,0,w]</td>
<td>0,x,0 [0,u,w]</td>
</tr>
<tr>
<td>4 k .2'</td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
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<tr>
<td>4 j .2'</td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
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<tr>
<td>4 i 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
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<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<tr>
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<td>0,1/2,1/2 [0,0,w]</td>
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<td>2 e 22'2'</td>
<td>1/2,0,0 [0,0,w]</td>
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<td>0,1/2,0 [0,0,w]</td>
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<tr>
<td>1 d 42'2'</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
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<td>1 c 42'2'</td>
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<td>1/2,1/2,0 [0,0,w]</td>
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<tr>
<td>1 b 42'2'</td>
<td>0,0,1/2 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2'2'm'
a* = -c  b* = b
Origin at x,0,0

Along [1,1,0] p2'2'm'
a* = -c  b* = (-a + b)/2
Origin at x,x,0
Origin on 4'2'2

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
   (1|0,0,0)

(2) 2’ 0,0,z
    (2_z|0,0,0)

(3) 4’’’ 0,0,z
    (4_z|0,0,0)'

(4) 4’’’ 0,0,z
    (4_z|0,0,0)'

(5) 2’ 0,y,0
    (2_y|0,0,0)'

(6) 2’’ x,0,0
    (2_x|0,0,0)'

(7) 2’ x,x,0
    (2_y|x,0,0)

(8) 2’’’ x,x,0
    (2_y|x,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

8 p 1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w]
(5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w]

4 o .2'. x,1/2,0 [0,v,w] x,1/2,0 [0,v,w] 1/2,x,0 [v,0,w] 1/2,x,0 [v,0,w]
4 n .2'. x,0,1/2 [0,v,w] x,0,1/2 [0,v,w] 0,x,1/2 [v,0,w] 0,x,1/2 [v,0,w]
4 m .2'. x,1/2,1/2 [0,v,w] x,1/2,1/2 [0,v,w] 1/2,x,1/2 [v,0,w] 1/2,x,1/2 [v,0,w]
4 l .2'. x,0,0 [0,v,w] x,0,0 [0,v,w] 0,x,0 [v,0,w] 0,x,0 [v,0,w]
4 k ..2 x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0]
4 j ..2 x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0]
4 i 2.. 0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z [0,0,w]
2 h 4'.. 1/2,1/2,z [0,0,0] 1/2,1/2,z [0,0,0] 0,0,z [0,0,0] 0,0,z [0,0,0]
2 g 4'.. 0,0,z [0,0,0] 0,0,z [0,0,0] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w]
2 f 22'2'. 1/2,0,1/2 [0,0,w] 0,1/2,1/2 [0,0,w] 0,1/2,1/2 [0,0,w] 0,1/2,1/2 [0,0,w]
2 e 22'2'. 1/2,0,0 [0,0,w] 0,1/2,0 [0,0,w] 0,1/2,0 [0,0,w] 0,1/2,0 [0,0,w]
1 d 4'2' 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]
1 c 4'2' 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]
1 b 4'2' 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0]
1 a 4'2' 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4'm'm
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2'mm'
a* = -c  b* = b
Origin at x,0,0

Along [1,1,0] p2'mm'
a* = -c  b* = (-a + b)/2
Origin at x,x,0
Origin on 422

Asymmetric unit: $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
2. $2 \cdot 0,0,z$
3. $4^+ \cdot 0,0,z$
4. $4^- \cdot 0,0,z$
5. $2 \cdot 0,y,0$
6. $2 \cdot x,0,0$
7. $2 \cdot x,x,0$
8. $2 \cdot x,x,0$

For $(0,0,1)' +$ set

1. $1'$
2. $2' \cdot 0,0,1'$
3. $4^+ \cdot (0,0,1)' 0,0,1'$
4. $4^- \cdot (0,0,1)' 0,0,1'$
5. $2' \cdot 0,y,1/2$
6. $2' \cdot x,0,1/2$
7. $2' \cdot x,x,1/2$
8. $2' \cdot x,x,1/2$
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 p 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w] (5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 o .2.</td>
<td>x,1/2,0 [u,0,0] x,1/2,0 [u,0,0] 1/2,x,0 [0,u,0] 1/2,x,0 [0,u,0]</td>
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<tr>
<td>8 n .2'</td>
<td>x,0,1/2 [0,v,w] x,0,1/2 [0,v,w] 0,x,1/2 [v,0,w] 0,x,1/2 [v,0,w]</td>
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<tr>
<td>8 m .2'</td>
<td>x,1/2,1/2 [0,v,w] x,1/2,1/2 [0,v,w] 1/2,x,1/2 [v,0,w] 1/2,x,1/2 [v,0,w]</td>
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<tr>
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<tr>
<td>8 k ..2'</td>
<td>x,x,1/2 [u,u,w] x,x,1/2 [u,u,w] x,x,1/2 [u,u,w] x,x,1/2 [u,u,w]</td>
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<tr>
<td>8 j ..2</td>
<td>x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>8 i 2..</td>
<td>0,1/2,0 [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 h 4..</td>
<td>1/2,1/2,2 [0,0,w] 1/2,1/2,2 [0,0,w] 1/2,1/2,2 [0,0,w] 1/2,1/2,2 [0,0,w]</td>
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<tr>
<td>4 g 4..</td>
<td>0,0,2 [0,0,w] 0,0,2 [0,0,w] 0,0,2 [0,0,w] 0,0,2 [0,0,w]</td>
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<tr>
<td>4 f 22'2'.</td>
<td>1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w]</td>
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<tr>
<td>4 e 222.</td>
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<tr>
<td>2 d 42'2'</td>
<td>1/2,1/2,1/2 [0,0,w] 1/2,1/2,1/2 [0,0,w] 1/2,1/2,1/2 [0,0,w] 1/2,1/2,1/2 [0,0,w]</td>
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<tr>
<td>2 c 422</td>
<td>1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>2 b 42'2'</td>
<td>0,0,1/2 [0,0,w] 0,0,1/2 [0,0,w] 0,0,1/2 [0,0,w] 0,0,1/2 [0,0,w]</td>
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<tr>
<td>2 a 422</td>
<td>0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p4mm1'</td>
<td>a* = a b* = b</td>
</tr>
<tr>
<td>Along [1,0,0] p2a'2m'm'</td>
<td>a* = c b* = b</td>
</tr>
<tr>
<td>Along [1,1,0] p2a'2m'm'</td>
<td>a* = c b* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,0,0] p2a'2m'm'</td>
<td>a* = c b* = b</td>
</tr>
<tr>
<td>Along [1,1,0] p2a'2m'm'</td>
<td>a* = c b* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 422

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. 1
2. 2, 0, 0, z
   - $(2z, 0, 0, 0)$
3. 4*, 0, 0, z
   - $(4z, 0, 0, 0)$
4. 4*, 0, 0, z
   - $(4z^{-1}, 0, 0, 0)$

For $(1,0,0)'$ + set

1. $(1,0,0)'$
2. $2', 1/2, 0, z$
   - $(2z, 1, 0, 0)^r$
3. $4', 1/2, 1/2, z$
   - $(4z, 1, 0, 0)^r$
4. $4', 1/2, -1/2, z$
   - $(4z^{-1}, 1, 0, 0)^r$
## Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 p</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
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<td></td>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 o</td>
<td>.2'</td>
<td>x,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,1/2,0 [0,v,w]</td>
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<td>8 n</td>
<td>.2</td>
<td>x,0,1/2 [u,0,0]</td>
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<tr>
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<td></td>
<td>(7) x,0,1/2 [u,0,0]</td>
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<tr>
<td>8 m</td>
<td>.2'</td>
<td>x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) x,1/2,1/2 [0,v,w]</td>
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<tr>
<td>8 l</td>
<td>.2</td>
<td>x,0,0 [u,0,0]</td>
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<td>(9) x,0,0 [u,0,0]</td>
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<tr>
<td>8 k</td>
<td>.2</td>
<td>x,x,1/2 [u,u,0]</td>
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<td></td>
<td>(10) x,x,1/2 [u,u,0]</td>
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<tr>
<td>8 j</td>
<td>.2</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
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<td></td>
<td>(11) x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>2'</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) 0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 h</td>
<td>4'</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(13) 1/2,1/2,z [0,0,0]</td>
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<tr>
<td>4 g</td>
<td>4</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(14) 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 f</td>
<td>2'22'</td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(15) 1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 e</td>
<td>2'22'</td>
<td>1/2,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(16) 1/2,0,0 [u,0,0]</td>
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<tr>
<td>2 d</td>
<td>4'2'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c</td>
<td>4'2'</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b</td>
<td>422</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a</td>
<td>422</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

## Coordinates

<table>
<thead>
<tr>
<th>(0,0,0) +</th>
<th>(1,0,0)' +</th>
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<tbody>
<tr>
<td>x,y,z</td>
<td>x,y,z</td>
</tr>
<tr>
<td>x,y,z</td>
<td>x,y,z</td>
</tr>
<tr>
<td>y,x,z</td>
<td>y,x,z</td>
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<tr>
<td>y,x,z</td>
<td>y,x,z</td>
</tr>
<tr>
<td>x,y,z</td>
<td>x,y,z</td>
</tr>
<tr>
<td>x,1/2,0</td>
<td>1/2,x,0</td>
</tr>
<tr>
<td>0,x,1/2</td>
<td>0,x,1/2</td>
</tr>
<tr>
<td>x,1/2,1/2</td>
<td>1/2,x,1/2</td>
</tr>
<tr>
<td>0,x,0</td>
<td>0,x,0</td>
</tr>
<tr>
<td>x,x,1/2</td>
<td>x,x,1/2</td>
</tr>
<tr>
<td>x,x,0</td>
<td>x,x,0</td>
</tr>
<tr>
<td>0,1/2,z</td>
<td>0,1/2,z</td>
</tr>
<tr>
<td>0,1/2,z</td>
<td>1/2,0,z</td>
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<td>0,0,z</td>
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<td>0,1/2,z</td>
<td>1/2,0,z</td>
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<td>0,1/2,z</td>
<td>1/2,0,z</td>
</tr>
</tbody>
</table>

## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,1/2,z</th>
<th>Origin at x,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>a* = b</td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>a* = (-a + b)/2</td>
<td>a* = b</td>
</tr>
<tr>
<td>b* = c</td>
<td>b* = b</td>
</tr>
</tbody>
</table>
Origin on 422

Asymmetric unit  \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
   \((1|0,0,0)\)
2. \(2\) 0,0,z
   \((2_z|0,0,0)\)
3. \(4^+\) 0,0,z
   \((4_z|0,0,0)\)
4. \(4^-\) 0,0,z
   \((4_z^{-1}|0,0,0)\)
5. 2 0,y,0
   \((2_y|0,0,0)\)
6. 2 x,0,0
   \((2_x|0,0,0)\)
7. 2 x,x,0
   \((2_{xy}|0,0,0)\)
8. 2 x,\(\bar{x}\),0
   \((2_{xy}|0,0,0)\)

For \((1,0,0)\)' + set

1. \(t'\) (1,0,0)
   \((1|0,0,0)\)'
2. \(2'\) 1/2,0,z
   \((2_z|1,0,0)\)'
3. \(4'^+\) 1/2,1/2,z
   \((4_z|1,0,0)\)'
4. \(4'^-\) 1/2,-1/2,z
   \((4_z^{-1}|1,0,0)\)'
5. 2' 1/2,y,0
   \((2_y|1,0,0)\)'
6. 2' (1,0,0) x,0,0
   \((2_z|1,0,0)\)'
7. 2' (1/2,1/2,0) x+1/2,x,0
   \((2_{xy}|1,0,0)\)'
8. 2' (1/2,-1/2,0) x+1/2,\(\bar{x}\),0
   \((2_{xy}|1,0,0)\)'
**Generators selected**  
(1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**  

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
</tr>
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<td>(0,0,0) +</td>
<td>(1,0,0) +</td>
<td></td>
</tr>
<tr>
<td>16 p 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
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<td>(2) x,y,z [u,v,w]</td>
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<tr>
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<td>(3) x,y,z [v,u,w]</td>
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</tr>
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<td>(4) x,y,z [v,u,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<td>(6) x,y,z [u,v,w]</td>
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<td>(7) x,y,z [v,u,w]</td>
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<td>(8) x,y,z [v,u,w]</td>
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<tr>
<td>8 o .2'</td>
<td>x,1/2,0 [0,v,w]</td>
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<tr>
<td>8 n .2'</td>
<td>x,1/2,0 [0,v,w]</td>
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<tr>
<td>8 m .2</td>
<td>x,1/2,0 [0,v,w]</td>
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<td>8 l .2</td>
<td>x,1/2,0 [0,v,w]</td>
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<td>x,1/2,0 [0,v,w]</td>
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<tr>
<td>8 j .2</td>
<td>x,1/2,0 [0,v,w]</td>
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</tr>
<tr>
<td>8 i .2</td>
<td>x,1/2,0 [0,v,w]</td>
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</tr>
<tr>
<td>4 h 4'</td>
<td>x,1/2,0 [0,v,w]</td>
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<tr>
<td>4 g 4'</td>
<td>x,1/2,0 [0,v,w]</td>
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<td>4 f 2'</td>
<td>x,1/2,0 [0,v,w]</td>
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<tr>
<td>4 e 2'</td>
<td>x,1/2,0 [0,v,w]</td>
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</tr>
<tr>
<td>2 d 2'</td>
<td>x,1/2,0 [0,v,w]</td>
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</tr>
<tr>
<td>2 c 2'</td>
<td>x,1/2,0 [0,v,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 2'</td>
<td>x,1/2,0 [0,v,w]</td>
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<tr>
<td>2 a 2'</td>
<td>x,1/2,0 [0,v,w]</td>
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</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1'</th>
<th>Along [1,0,0] p2mm1'</th>
<th>Along [1,1,0] p–2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x-1/4,x+1/4,1/2</td>
</tr>
</tbody>
</table>
Origin on 4'22'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

1. 1  
   (1 | 0,0,0)
2. 2  0,0,z  
   (2z | 0,0,0)
3. 4'  0,0,z  
   (4z | 0,0,0)'
4. 4'  0,0,z  
   (4z⁻¹ | 0,0,0)'
5. 2  0,y,0  
   (2y | 0,0,0)
6. 2  x,0,0  
   (2x | 0,0,0)
7. 2'  x,x,0  
   (2xy | 0,0,0)'
8. 2'  x,x,0  
   (2xy | 0,0,0)'

For (0,0,1) + set

1'. (0,0,1)  
   (1 | 0,0,1)'
2'. (0,0,1)  0,0,z  
   (2z | 0,0,1)'
3. 4'  (0,0,1)  0,0,z  
   (4z | 0,0,1)
4. 4'  (0,0,1)  0,0,z  
   (4z⁻¹ | 0,0,1)
5'. 0,y,1/2  
   (2y | 0,0,1)'
6'. x,0,1/2  
   (2x | 0,0,1)'
7. 2'  x,x,1/2  
   (2xy | 0,0,1)
8. 2'  x,x,1/2  
   (2xy | 0,0,1)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1') +</td>
<td></td>
</tr>
<tr>
<td>16 p 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(4) y,x,z [v,u,w]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>8 o .2. x,1/2,0 [u,0,0]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 n .2'. x,0,1/2 [0,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 m .2'. x,1/2,1/2 [0,v,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 l .2. x,0,0 [u,0,0]</td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 k .2 x,x,1/2 [u,u,0]</td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 j .2' x,x,0 [u,u,w]</td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 i 2.. 0,1/2,z [0,0,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 h .2' 1/2,1/2,z [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>4 g .2' 0,0,z [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>4 f 22'2'. 1/2,0,1/2 [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>4 e 222'. 1/2,0,0 [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>2 d 4'22' 1/2,1/2,1/2 [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>2 c 4'22' 1/2,1/2,0 [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>2 b 4'22' 0,0,1/2 [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
<tr>
<td>2 a 4'22' 0,0,0 [0,0,0]</td>
<td>(0,0,0) + (0,0,1') +</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a</td>
<td>b' = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p_2c 2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a'^* = -c</td>
<td>b'^* = b</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p_2c 2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a'^* = -c</td>
<td>b'^* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at x,x,1/2</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 4'22'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $(1,0,0)$
2. $2 \cdot 0,0,z$
3. $4' \cdot 0,0,z$
4. $4' \cdot 0,0,z$

For $(1,0,0)'$ + set

1. $t'(1,0,0)$
2. $2' \cdot 1/2,0,z$
3. $4' \cdot 1/2,1/2,z$
4. $4' \cdot 1/2,-1/2,z$

5. $2' \cdot 1/2,y,0$
6. $2' \cdot (1,0,0)$
7. $2 (1/2,1/2,0)$
8. $2 (1/2,-1/2,0)$

$P_\text{p}4'22'$

4221'

Tetragonal

89.10.756

$P_\text{p}4'22'$

89.10.756 - 1 - 1504
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 p</td>
<td>1</td>
<td>((1)) (x,y,z) [(u,v,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((2)) (x',y',z) [(u',v',w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((3)) (y,x,z) [(v,u,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((4)) (y',x,z) [(v',u,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((5)) (x,y,z) [(u,v,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((6)) (x,y,z) [(u,v,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((7)) (y,x,z) [(v,u,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>((8)) (y,x,z) [(v,u,w)]</td>
</tr>
</tbody>
</table>

Coordinates

\[(0,0,0) + (1,0,0)' + (0,0,1)\]

\[\begin{array}{llll}
8 o & .2'. & x,1/2,0 & [0,v,w] \\
8 n & .2.  & x,0,1/2 & [u,0,0] \\
8 m & .2'. & x,1/2,1/2 & [v,w] \\
8 l & .2.  & x,0,0  & [u,0,0] \\
8 k & .2'. & x,x,1/2 & [u,u,0] \\
8 j & .2'. & x,x,0   & [u,u,0] \\
8 i & .2'.. & 0,1/2,z & [v,u,0] \\
4 h & .4..  & 1/2,1/2,z & [0,0,w] \\
4 g & .4'.. & 0,0,z   & [0,0,0] \\
4 f & 2'22' & 1/2,0,1/2 & [u,0,0] \\
4 e & 2'22' & 1/2,0,0  & [u,0,0] \\
2 d & 42'2' & 1/2,1/2,1/2 & [0,0,w] \\
2 c & 42'2' & 1/2,1/2,0 & [0,0,w] \\
2 b & 4'22' & 0,0,1/2 & [0,0,0] \\
2 a & 4'22' & 0,0,0   & [0,0,0] \\
\end{array}\]

Symmetry of Special Projections

Along [0,0,1] \(p_{p^*4mm}\)  
Along [1,0,0] \(p2mm1'\)  
Along [1,1,0] \(p_{2a^*2mm}\)

\[\begin{array}{lll}
a^* = a & b^* = b & \text{Origin at } 1/2,1/2,z \\
a^* = b & b^* = c & \text{Origin at } x,0,0 \\
a^* = (-a + b)/2 & b^* = c & \text{Origin at } x-1/4,x+1/4,0 \\
\end{array}\]
Origin at 222 at 212

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 \(0,0,z\)
(2 \(z\) | 0,0,0)

(3) 4 \(z\) \(0,1/2,z\)
(4 \(z\) | 1/2,1/2,0)

(4) 4 \(z\) \(1/2,0,z\)
(4 \(z\) | 1/2,1/2,0)

(5) 2 \(0,1/2,0\) \(1/4,y,0\)
(2 \(y\) | 1/2,1/2,0)

(6) 2 (1/2,0,0) \(x,1/4,0\)
(2 \(x\) | 1/2,1/2,0)

(7) 2 \(x,x,0\)
(2 \(x\) | 0,0,0)

(8) 2 \(x,x,0\)
(2 \(x\) | 0,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y+1/2,x+1/2,z [v,u,w]  (4) y+1/2,x+1/2,z [v,u,w]  (5) x+1/2,y+1/2,z [u,v,w]  (6) x+1/2,y+1/2,z [u,v,w]  (7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 f .2</td>
<td>x,x,1/2 [u,u,0]  x,x,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]</td>
</tr>
<tr>
<td>4 e .2</td>
<td>x,x,0 [u,u,0]  x,x,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]</td>
</tr>
<tr>
<td>4 d .2</td>
<td>0,0,z [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]  0,0,z [0,0,w]  0,0,z [0,0,w]  0,0,z [0,0,w]  0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 c 4..</td>
<td>0,1/2,z [0,0,w]  0,1/2,z [0,0,w]  1/2,0,1/2 [0,0,w]  1/2,0,1/2 [0,0,w]  1/2,0,1/2 [0,0,w]  1/2,0,1/2 [0,0,w]  1/2,0,1/2 [0,0,w]  1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 2.22</td>
<td>0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 2.22</td>
<td>0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4g'm'  Along [1,0,0] p2m'g'  Along [1,1,0] p2m'm'
\(a^* = a \quad b^* = b\)  \(a^* = b \quad b^* = c\)  \(a^* = (-a + b)/2 \quad b^* = c\)
Origin at 0,1/2,z  Origin at x,1/4,0  Origin at x,x,0
**Origin** at 2221' at 2121'

**Asymmetric unit**

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2} \]

**Symmetry Operations**

For \( 1 + \) set

1. \( 1 \)  \( (1 | 0,0,0) \)
2. \( 2 \)  \( 0,0,z \)  \( (2_z | 0,0,0) \)
3. \( 4^+ \)  \( 0,1/2,z \)  \( (4_z | 1/2,1/2,0) \)
4. \( 4^- \)  \( 1/2,0,z \)  \( (4_z^{-1} | 1/2,1/2,0) \)
5. \( 2 \)  \( (0,1/2,0) \)  \( 1/4,y,0 \)  \( (2_y | 1/2,1/2,0) \)
6. \( 2 \)  \( (1/2,0,0) \)  \( x,1/4,0 \)  \( (2_x | 1/2,1/2,0) \)
7. \( 2 \)  \( x,x,0 \)  \( (2_{xy} | 0,0,0) \)
8. \( 2 \)  \( x,0,0 \)  \( (2_{xy} | 0,0,0) \)

For \( 1' + \) set

1. \( 1' \)  \( (1 | 0,0,0)' \)
2. \( 2' \)  \( 0,0,z \)  \( (2_z | 0,0,0)' \)
3. \( 4'^+ \)  \( 0,1/2,z \)  \( (4_z | 1/2,1/2,0)' \)
4. \( 4'^- \)  \( 1/2,0,z \)  \( (4_z^{-1} | 1/2,1/2,0)' \)
5. \( 2' \)  \( (0,1/2,0) \)  \( 1/4,y,0 \)  \( (2_y | 1/2,1/2,0)' \)
6. \( 2' \)  \( (1/2,0,0) \)  \( x,1/4,0 \)  \( (2_x | 1/2,1/2,0)' \)
7. \( 2' \)  \( x,x,0 \)  \( (2_{xy} | 0,0,0)' \)
8. \( 2' \)  \( x,0,0 \)  \( (2_{xy} | 0,0,0)' \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x',y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z [0,0,0]</td>
<td>(4) y+1/2,x+1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [0,0,0]</td>
<td>(6) x+1/2,y+1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [0,0,0]</td>
<td>(8) y,x,z [0,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 f .21'</td>
<td>x,x,1/2 [0,0,0]</td>
<td>x',x,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [0,0,0]</td>
<td>x',x,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x+1/2,1/2 [0,0,0]</td>
<td>x+1/2,x+1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p4gm1'</td>
</tr>
<tr>
<td>a* = a  b* = b</td>
</tr>
<tr>
<td>Origin at 0,1/2,z</td>
</tr>
<tr>
<td>Along [1,0,0] p2mg1'</td>
</tr>
<tr>
<td>a* = b  b* = c</td>
</tr>
<tr>
<td>Origin at x,1/4,0</td>
</tr>
<tr>
<td>Along [1,1,0] p2mm1'</td>
</tr>
<tr>
<td>a* = (-a + b)/2  b* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin at 22'2' at 212'

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
(2) 2 0,0,z
    (2z 0,0,0)
(3) 4' 0,1/2,z
    (4z 1/2,1/2,0')
(4) 4' 1/2,0,z
    (4z -1 1/2,1/2,0')
(5) 2 (0,1/2,0) 1/4,y,0
    (2y 1/2,1/2,0)
(6) 2 (1/2,0,0) x,1/4,0
    (2x 1/2,1/2,0)
(7) 2' x,x,0
    (2xy 0,0,0')
(8) 2' x,x,0
    (2xy 0,0,0')
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) y,x+1/2,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) y,x+1/2,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) x,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(6) x,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

| 4 f ..2'     | x,x,1/2 [u,u,w]      |               |
| 4 e ..2'     | x,x,0 [u,u,w]        |               |
| 4 d 2..      | 0,0,z [0,0,w]        |               |
| 2 c 4'..     | 0,1/2,z [0,0,0]      |               |
| 2 b 2.2'2'   | 0,0,1/2 [0,0,w]      |               |
| 2 a 2.2'2'   | 0,0,0 [0,0,w]        |               |

### Symmetry of Special Projections

- Along [0,0,1]  p4'g'm
- Along [1,0,0]  p2m'g'
- Along [1,1,0]  p2m'm'

**a* = a  b* = b**

Origin at 0,1/2,z

**a* = b  b* = c**

Origin at x,1/4,0

**a* = (-a + b)/2  b* = c**

Origin at x,x,0
Origin at $22'2'$ at $212'$

Asymmetric unit $0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/2$

Symmetry Operations

(1) 1
(1) $0,0,0$

(2) $2 \cdot 0,0,z$
(2) $z_{z}0,0,0$

(3) $4^* \cdot 0,1/2,z$
(3) $z_{z}1/2,1/2,0$

(4) $4^* \cdot 1/2,0,z$
(4) $z_{z}1/2,1/2,0$

(5) $2' \cdot 0,1/2,0$
(5) $x,y,0$

(6) $2' (1/2,0,0)$
(6) $x,1/4,0$

(7) $2' \cdot x,x,0$
(7) $x,0,0$

(8) $2' \cdot x,x,0$
(8) $x,0,0$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
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<td>(3) y+1/2,x+1/2,z [v,u,w]</td>
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<td>4</td>
<td>f ..2' x,x,1/2 [u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
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<td>x+1/2,x+1/2,1/2 [u,u,w]</td>
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<td>e ..2' x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
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<td>d 2.. 0,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
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<td></td>
<td>0,0,z [0,0,w]</td>
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<tr>
<td>2</td>
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</tr>
<tr>
<td>2</td>
<td>b 2.2'2' 0,0,1/2 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
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<tr>
<td>2</td>
<td>a 2.2'2' 0,0,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm  Along [1,0,0] p2m'g'  Along [1,1,0] p2mm'
\( a^* = a \)  \( b^* = b \)  \( a^* = -c \  \) \( b^* = (-a + b)/2 \)
Origin at 0,1/2,z  Origin at x,1/4,0  Origin at x,x,0
Origin at 222 at 212

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations:

1. $1$
   
2. $2 \quad 0,0,z$
   
3. $4' \quad 0,1/2,z$

4. $4' \quad 1/2,0,z$
   
5. $2' (0,1/2,0) \quad 1/4,y,0$
   
6. $2' (1/2,0,0) \quad x,1/4,0$
   
7. $2 \quad x,x,0$
   
8. $2 \quad x,x,0$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordination</th>
<th>Coordinates</th>
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<tbody>
<tr>
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<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z [v,u,w]</td>
<td>(4) y+1/2,x+1/2,z [v,u,w]</td>
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<tr>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
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<tr>
<td>4 f 2</td>
<td>x,x,1/2 [u,u,0]</td>
<td>x,x,1/2 [u,u,0]</td>
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<td>x+1/2,x+1/2,1/2 [u,u,0]</td>
<td>x+1/2,x+1/2,1/2 [u,u,0]</td>
</tr>
<tr>
<td>4 e 2</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
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<td>x+1/2,x+1/2,0 [u,u,0]</td>
</tr>
<tr>
<td>4 d 2</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
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<td>1/2,1/2,0 [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 c 4'</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 b 2.22</td>
<td>0,0,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 2.22</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p4'gm'  
  \[ a^* = a \quad b^* = b \]
  Origin at 0,1/2,z

- **Along [1,0,0]**: p2m'g'  
  \[ a^* = b \quad b^* = c \]
  Origin at x,1/4,0

- **Along [1,1,0]**: p2mm'  
  \[ a^* = -c \quad b^* = (-a + b)/2 \]
  Origin at x,x,0
Origin at 222 at 212

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0)\) + set

1. \((1,0,0,0)\)
2. \((2,0,0,z)\) \((2z,0,0,0)\)
3. \((4,0,1/2,z)\) \((4z,1/2,1/2,0)\)
4. \((4,1/2,0,z)\) \((4z^{-1},1/2,1/2,0)\)

For \((0,0,1)\) + set

1. \((t,0,0,1)\) \((t,0,0,1)'\)
2. \((2',0,0,1)\) \((2z,0,0,1)'\)
3. \((4\,4',0,0,1)\) \((0,1/2,z)\) \((4z,1/2,1/2,0)\)
4. \((4\,4',0,0,1)\) \((0,1/2,0,z)\) \((4z^{-1},1/2,1/2,0)\)
Continued

90.6.762

\[ \text{P}_{\text{2c}} \ 421, \ 2 \]

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g (1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>(2) ( x,\bar{y},z ) [\bar{u},\bar{v},w]</td>
<td></td>
</tr>
<tr>
<td>(3) ( y+1/2,x+1/2,z ) [\bar{v},u,w]</td>
<td></td>
</tr>
<tr>
<td>(4) ( y+1/2,x+1/2,z ) [v,\bar{u},w]</td>
<td></td>
</tr>
<tr>
<td>(5) ( x+1/2,y+1/2,z ) [u,\bar{v},w]</td>
<td></td>
</tr>
<tr>
<td>(6) ( x+1/2,y+1/2,z ) [u,v,\bar{w}]</td>
<td></td>
</tr>
<tr>
<td>(7) ( y,x,z ) [v,u,\bar{w}]</td>
<td></td>
</tr>
<tr>
<td>(8) ( y,x,z ) [v,\bar{u},w]</td>
<td></td>
</tr>
</tbody>
</table>

8 f '..2' x,x,1/2 \[u,u,w\]  
8 e '..2 x,x,0 \[u,u,0\]  
8 d 2.. 0,0,z \[0,0,w\]  
4 c 4.. 0,1/2,z \[0,0,w\]  
4 b 2.2'2' 0,0,1/2 \[0,0,w\]  
4 a 2.22 0,0,0 \[0,0,0\]  

### Symmetry of Special Projections

- **Along [0,0,1]** p4gm1'  
  \( a^* = a \quad b^* = b \)  
  Origin at 0,1/2,z

- **Along [1,0,0]** p2m'g'  
  \( a^* = b \quad b^* = c \)  
  Origin at x,1/4,0

- **Along [1,1,0]** P_{2c'} 2m'm'  
  \( a^* = -c \quad b^* = (-a + b)/2 \)  
  Origin at x,x,0
Origin at 222 at 212

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For (0,0,0) + set

1. $1$
2. $2' \ (0,0,0) \quad 0,0,z$
3. $4' \ (0,0,0) \quad 0,0,z$
4. $4' \ (0,0,0) \quad 0,0,z$

5. $2' \ (0.1/2,0) \quad 1/4,y,0$
6. $2' \ (1/2,0,0) \quad x,1/4,0$
7. $2 \ (0,1/2,0) \quad 1/4,y,0$
8. $2 \ (1/2,0,0) \quad x,1/4,0$

For (0,0,1)' + set

1. $t' \ (0,0,1)$
2. $2' \ (0,0,1) \quad 0,0,z$
3. $4' \ (0,0,1) \quad 0,1/2,z$
4. $4' \ (0,0,1) \quad 0,1/2,z$

5. $2 \ (0.1/2,0) \quad 1/4,y,1/2$
6. $2 \ (1/2,0,0) \quad x,1/4,1/2$
7. $2' \ (0,0,1)' \quad 0,0,z$
8. $2' \ (0,0,1)' \quad 0,0,z$
Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td>1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y+1/2,x+1/2,z [v,u,w] (4) y+1/2,x+1/2,z [v,u,w] (5) x+1/2,y+1/2,z [u,v,w] (6) x+1/2,y+1/2,z [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 f</td>
<td>.2'</td>
<td>x,x,1/2 [u,u,w] x,x,1/2 [u,u,w] x+1/2,x+1/2,1/2 [u,u,w] x+1/2,x+1/2,1/2 [u,u,w] x+1/2,x+1/2,1/2 [u,u,w]</td>
</tr>
<tr>
<td>8 e</td>
<td>.2</td>
<td>x,x,0 [u,u,0] x,x,0 [u,u,0] x+1/2,x+1/2,0 [u,u,0] x+1/2,x+1/2,0 [u,u,0]</td>
</tr>
<tr>
<td>8 d</td>
<td>2..</td>
<td>0,0,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 c</td>
<td>4'..</td>
<td>0,1/2,z [0,0,0] 1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>2.2'2'</td>
<td>0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>2.22</td>
<td>0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1' a* = a  b* = b
Along [1,0,0] p2m'g' a* = b  b* = c
Along [1,1,0] p222 2m'm' a* = -c  b* = (-a + b)/2
Origin at 0,1/2,z Origin at x,1/4,0 Origin at x,x,0
Origin on 2 [0 1 0] at 4, (1,2) 1

Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

(1) 1 (1) 0,0,0
(1) 0,0,0

(2) 2 (0,0,1/2) 0,0,z
(2) 0,0,1/2

(3) 4^+ (0,0,1/4) 0,0,z
(4) 4^- (0,0,1/4) 0,0,z

(4)^- (0,0,3/4) 0,0,z
(4)^+ (0,0,3/4)

(5) 2 0,y,0
(2z|0,0,0)

(6) 2 x,0,1/4
(2z|0,0,1/2)

(7) 2 x,x,3/8
(2xy|0,0,3/4)

(8) 2 x,x,1/8
(2xy|0,0,1/4)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
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<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<tr>
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<td>(3) y,x,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<tr>
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<td>(6) x,y,z+1/2 [u,v,w]</td>
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<tr>
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<td>(7) y,x,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z+1/4 [v,u,w]</td>
</tr>
</tbody>
</table>

| 4 c ..2      | x,x,7/8 [u,u,0] |
|              | x,x,5/8 [u,u,0] |
|              | x,x,1/8 [u,u,0] |

| 4 b .2       | 1/2,y,0 [0,v,0] |
|              | 1/2,y,1/2 [0,v,0] |
|              | y,1/2,1/4 [v,0,0] |
|              | y,1/2,3/4 [v,0,0] |

| 4 a .2       | 0,y,0 [0,v,0] |
|              | 0,y,1/2 [0,v,0] |
|              | y,0,1/4 [v,0,0] |
|              | y,0,3/4 [v,0,0] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4m'm'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at x,0,1/4</td>
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<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c</td>
<td>b* = (-a + b)/2</td>
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<tr>
<td>Origin at x,x,3/8</td>
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</tbody>
</table>
Origin on 21' [0 1 0 ] at 4, (1,2) 11'

Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

For 1 + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
<th>Symmetry Element</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(1</td>
<td>0,0,0)</td>
</tr>
<tr>
<td>(2) 2</td>
<td>(0,0,1/2) 0,0,z</td>
<td></td>
</tr>
<tr>
<td>(3) 4'</td>
<td>(0,0,1/4) 0,0,z</td>
<td></td>
</tr>
<tr>
<td>(4) 4''</td>
<td>(0,0,1/4) 0,0,z</td>
<td></td>
</tr>
<tr>
<td>(5) 2'</td>
<td>(0,0,0)</td>
<td>(2y</td>
</tr>
<tr>
<td>(6) 2''</td>
<td>x,0,1/4</td>
<td>(2y</td>
</tr>
<tr>
<td>(7) 2'''</td>
<td>x,x,3/8</td>
<td>(2y</td>
</tr>
<tr>
<td>(8) 2''''</td>
<td>x,x,1/8</td>
<td>(2y</td>
</tr>
</tbody>
</table>

For 1' + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
<th>Symmetry Element</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1'</td>
<td>(1</td>
<td>0,0,0)'</td>
</tr>
<tr>
<td>(2) 2'</td>
<td>(0,0,1/2) 0,0,z</td>
<td></td>
</tr>
<tr>
<td>(3) 4''</td>
<td>(0,0,1/4) 0,0,z</td>
<td></td>
</tr>
<tr>
<td>(4) 4'''</td>
<td>(0,0,1/4) 0,0,z</td>
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</tr>
<tr>
<td>(5) 2''</td>
<td>(0,0,0)'</td>
<td>(2y</td>
</tr>
<tr>
<td>(6) 2'''</td>
<td>x,0,1/4</td>
<td>(2y</td>
</tr>
<tr>
<td>(7) 2''''</td>
<td>x,x,3/8</td>
<td>(2y</td>
</tr>
<tr>
<td>(8) 2''''</td>
<td>x,x,1/8</td>
<td>(2y</td>
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Generators selected
(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>8 d 11'</td>
<td>(1) x,y,z [0,0,0]</td>
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<tr>
<td></td>
<td>(2) x,y,z+1/2 [0,0,0]</td>
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</tr>
<tr>
<td></td>
<td>(3) y,x,z+1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+3/4 [0,0,0]</td>
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<td></td>
<td>(5) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
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<td>(6) x,y,z+1/2 [0,0,0]</td>
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</tr>
<tr>
<td></td>
<td>(7) y,x,z+3/4 [0,0,0]</td>
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<tr>
<td></td>
<td>(8) y,x,z+1/4 [0,0,0]</td>
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<tr>
<td>4 c .21'</td>
<td>x,x,3/8 [0,0,0]</td>
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<tr>
<td></td>
<td>x,x,7/8 [0,0,0]</td>
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<td>x,x,5/8 [0,0,0]</td>
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<tr>
<td></td>
<td>x,x,1/8 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 b .21'</td>
<td>1/2,y,0 [0,0,0]</td>
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<tr>
<td></td>
<td>1/2,y,1/2 [0,0,0]</td>
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<tr>
<td></td>
<td>y,1/2,1/4 [0,0,0]</td>
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<tr>
<td></td>
<td>y,1/2,3/4 [0,0,0]</td>
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<tr>
<td>4 a .21'</td>
<td>0,y,0 [0,0,0]</td>
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<td>0,y,1/2 [0,0,0]</td>
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<td>y,0,1/4 [0,0,0]</td>
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<td>y,0,3/4 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4mm1'  Along [1,0,0] p2mg1'  Along [1,1,0] p2mg1'
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
\( \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)

Origin at 0,0,z  Origin at x,0,1/4  Origin at x,x,3/8
Origin on $\mathbf{2}$ [0 1 0] at $\mathbf{4}$, (1,2) 1

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

Symmetry Operations

1. $\mathbf{1}$
2. $\mathbf{2}$ (0, 0, 1/2) 0, 0, z
   $\mathbf{2}_z$ (0, 0, 1/2)
3. $\mathbf{4}$** (0, 0, 1/4) 0, 0, z
   $\mathbf{4}_z$ (0, 0, 1/4)
4. $\mathbf{4}$** (0, 0, 3/4) 0, 0, z
   $\mathbf{4}_z$ (0, 0, 3/4)
5. $\mathbf{2}$ 0, y, 0
   $\mathbf{2}_y$ (0, 0, 0)
6. $\mathbf{2}$ x, 0, 1/4
   $\mathbf{2}_x$ (0, 0, 1/2)
7. $\mathbf{2}$** x, x, 3/8
   $\mathbf{2}_x$ (0, 0, 3/4)
8. $\mathbf{2}$** x, x, 1/8
   $\mathbf{2}_x$ (0, 0, 1/4)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>8</th>
<th>d</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z+1/2 [u,v,w]</th>
<th>(3) y,x,z+1/4 [v,u,w]</th>
<th>(4) y,x,z+3/4 [v,u,w]</th>
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<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td>4</td>
<td>c</td>
<td>..2'</td>
<td>x,x,3/8 [u,u,w]</td>
<td>x,x,7/8 [u,u,w]</td>
<td></td>
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</tr>
<tr>
<td>4</td>
<td>b</td>
<td>.2</td>
<td>1/2,y,0 [0,v,0]</td>
<td>1/2,y,1/2 [0,v,0]</td>
<td>y,1/2,1/4 [v,0,0]</td>
<td>y,1/2,3/4 [v,0,0]</td>
</tr>
<tr>
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<td>a</td>
<td>.2</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
<td>y,0,1/4 [v,0,0]</td>
<td>y,0,3/4 [v,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4\nw'\n\n\n\na^* = a \quad b^* = b \\
\nOrigin at 0,0,z

Along [1,0,0] p2m'g'

\n\n\n\na^* = -c \quad b^* = b \\
\nOrigin at x,0,1/4

Along [1,1,0] p2'mg'

\n\n\n\na^* = -c \quad b^* = (-a + b)/2 \\
\nOrigin at x,x,3/8
Origin on $2' [0 1 0]$ at $4_1 (1, 2') 1$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/8$

Symmetry Operations

1. $1$
2. $2 (0,0,1/2) 0,0,z$
3. $4' (0,0,1/4) 0,0,z$
4. $4' (0,0,3/4) 0,0,z$
5. $2' 0,y,0$
6. $2' x,0,1/4$
7. $2' x,x,3/8$
8. $2' x,x,1/8$

$P4,2'2'$
$91.4.767$

$42'2'$
$P4,2'2'$

Tetragonal
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<td>(3) y,x,z+1/4 [v,u,w]</td>
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<td>(4) y,x,z+3/4 [v,u,w]</td>
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<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(7) y,x,z+3/4 [v,u,w]</td>
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<tr>
<td></td>
<td>(8) y,x,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>x,x,3/8 [u,u,w]</td>
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<td></td>
<td>x,x,7/8 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,5/8 [u,u,w]</td>
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<tr>
<td></td>
<td>x,x,1/8 [u,u,w]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,y,1/2 [u,0,w]</td>
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<tr>
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<td>y,1/2,1/4 [0,u,w]</td>
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<td>y,1/2,3/4 [0,u,w]</td>
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<tr>
<td>4 a .2'</td>
<td>0,y,0 [u,0,w]</td>
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<td></td>
<td>y,0,3/4 [0,u,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p2'mg'
\( a^* = -c \quad b^* = b \)
Origin at x,0,1/4

Along [1,1,0] p2'mg'
\( a^* = -c \quad b^* = (-a + b)/2 \)
Origin at x,x,3/8
Origin on 2' [0 1 0] at 4' (1,2') 1

Asymmetric unit
0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

(1) \begin{align*}
1 \\
1' (0,0,0)
\end{align*}

(1) \begin{align*}
1 \\
1' (0,0,0)
\end{align*}

(2) \begin{align*}
2' (0,0,1/2) \\
2' (0,0,1/2)
\end{align*}

(2) \begin{align*}
2' (0,0,1/2) \\
2' (0,0,1/2)
\end{align*}

(3) \begin{align*}
4' (0,0,1/4) \\
4' (0,0,1/4)
\end{align*}

(3) \begin{align*}
4' (0,0,1/4) \\
4' (0,0,1/4)
\end{align*}

(4) \begin{align*}
4'' (0,0,3/4) \\
4'' (0,0,3/4)
\end{align*}

(4) \begin{align*}
4'' (0,0,3/4) \\
4'' (0,0,3/4)
\end{align*}

(5) \begin{align*}
2' (0,y,0) \\
2' (0,y,0)
\end{align*}

(5) \begin{align*}
2' (0,y,0) \\
2' (0,y,0)
\end{align*}

(6) \begin{align*}
2 (x,0,1/4) \\
2 (x,0,1/4)
\end{align*}

(6) \begin{align*}
2 (x,0,1/4) \\
2 (x,0,1/4)
\end{align*}

(7) \begin{align*}
2 (x,x,3/8) \\
2 (x,x,3/8)
\end{align*}

(7) \begin{align*}
2 (x,x,3/8) \\
2 (x,x,3/8)
\end{align*}

(8) \begin{align*}
2 (x,x,1/8) \\
2 (x,x,1/8)
\end{align*}

(8) \begin{align*}
2 (x,x,1/8) \\
2 (x,x,1/8)
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z+1/2 [u,v,w] (3) y,x,z+1/4 [v,u,w] (4) y,x,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) y,x,z+3/4 [v,u,w] (8) y,x,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>4 c -2</td>
<td>x,x,3/8 [u,u,0] x,x,7/8 [u,u,0] x,x,5/8 [u,u,0] x,x,1/8 [u,u,0]</td>
</tr>
<tr>
<td>4 b 2'</td>
<td>1/2,y,0 [u,0,w] 1/2,y,1/2 [u,0,w] y,1/2,1/4 [0,u,w] y,1/2,3/4 [0,u,w]</td>
</tr>
<tr>
<td>4 a 2'</td>
<td>0,y,0 [u,0,w] 0,y,1/2 [u,0,w] y,0,1/4 [0,u,w] y,0,3/4 [0,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p4'mm'  
  \( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
  Origin at 0,0,z

- Along [1,0,0] p2'mg'  
  \( \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \)  
  Origin at x,0,1/4

- Along [1,1,0] p2m'g'  
  \( \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)  
  Origin at x,x,3/8
Origin on 2 [0 1 0] at 4, (1,2) 1

Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2 (0,0,1/2) 0,0,z
(2) 0,0,1/2

(3) 4’ (0,0,1/4) 0,0,z
(4) 0,0,1/4

(4) 4’ (0,0,3/4) 0,0,z
(4) 0,0,3/4

(5) 2' y,0,0
(2,0,0,0)

(6) 2' 0,0,1/4
(2,0,0,1/2)

(7) 2' x,x,3/8
(2,x,0,3/4)

(8) 2' x,y,1/8
(2,y,0,1/4)

For (1,0,0)' + set

(1) t' (1,0,0)
(1) 1,0,0'

(2) 2' (0,0,1/2) 1/2,0,z
(2) 1,0,1/2'

(3) 4’’ (0,0,1/4) 1/2,1/2,z
(4) 1,0,1/4’’

(4) 4’’ (0,0,3/4) 1/2,-1/2,z
(4) 1,0,3/4’’

(5) 2' 1/2,y,0
(2) 1/2,0,0'

(6) 2' (1,0,0) x,0,1/4
(2,1,0,1/2')

(7) 2' (1/2,1/2,0) x+1/2,x,3/8
(2,x,1,0,3/4’’)

(8) 2' (1/2,-1/2,0) x+1/2,x,1/8
(2,x,1,0,1/4’’)

91.6.769 - 1 - 1530
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

\begin{align*}
\text{Coordinates} & \\
(0,0,0) & \quad + & (1,0,0)' & \quad + \\
16 & d & 1 & (1) \begin{array}{c} x,y,z \ [u,v,w] \end{array} & (2) \begin{array}{c} \bar{x},\bar{y},\bar{z}+1/2 \ [\bar{u},\bar{v},\bar{w}] \end{array} & (3) \begin{array}{c} y,\bar{x},z+1/4 \ [\bar{v},u,w] \end{array} & (4) \begin{array}{c} y,\bar{x},z+3/4 \ [v,u,w] \end{array} \\
& & & (5) \begin{array}{c} \bar{x},\bar{y},\bar{z} \ [\bar{u},\bar{v},\bar{w}] \end{array} & (6) \begin{array}{c} x,\bar{y},\bar{z}+1/2 \ [u,\bar{v},\bar{w}] \end{array} & (7) \begin{array}{c} y,\bar{x},z+3/4 \ [v,u,\bar{w}] \end{array} & (8) \begin{array}{c} \bar{y},\bar{x},z+1/4 \ [\bar{v},u,\bar{w}] \end{array} \\
8 & c & .2 & x,x,3/8 \ [u,u,0] & \bar{x},\bar{x},7/8 \ [\bar{u},u,0] & \bar{x},x,5/8 \ [\bar{u},u,0] & x,\bar{x},1/8 \ [u,u,0] \\
8 & b & .2' & 1/2,y,0 \ [u,0,w] & 1/2,\bar{y},1/2 \ [u,0,w] & \bar{y},1/2,1/4 \ [0,u,w] & y,1/2,3/4 \ [0,u,\bar{w}] \\
8 & a & .2 & 0,y,0 \ [0,v,0] & 0,\bar{y},1/2 \ [0,v,0] & \bar{y},0,1/4 \ [\bar{v},0,0] & y,0,3/4 \ [v,0,0] \\
\end{align*}

Symmetry of Special Projections

\begin{align*}
\text{Along } [0,0,1] & \quad p_\varphi,4m'm' & \text{Along } [1,0,0] & \quad p2m1' & \text{Along } [1,1,0] & \quad p_{2\varphi},2m'g' \\
a^* = a & \quad b^* = b & \quad a^* = -c & \quad b^* = b & \quad a^* = -c & \quad b^* = (-a + b)/2 \\
\text{Origin at } 0,0,z & \quad \text{Origin at } x,0,1/4 & \quad \text{Origin at } x,x,3/8 \\
\end{align*}
Origin on 2 [0 1 0] at 4, (1,2) 1

Asymmetric unit  
0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

For (0,0,0) + set

1. 1  (0,0,0)  
2. 2 (0,0,1/2) 0,0,z  (2z,0,0,1/2)  
3. 4' (0,0,1/4) 0,0,z  (4z,0,0,1/4)'  
4. 4' (0,0,3/4) 0,0,z  (4z,0,0,3/4)'  

For (1,0,0)' + set

1'. (1,0,0)  
2' (0,0,1/2) 1/2,0,z  (2z,1,0,1/2)'  
3'. (0,0,1/4) 1/2,1/2,z  (4z,1,0,1/4)  
4'. (0,0,3/4) 1/2,-1/2,z  (4z,1,0,3/4)  

For (1,0,0)' + set

1. 1' (1,0,0)  
2' (0,0,1/2) 1/2,0,z  (2z,1,0,1/2)'  
3. 4' (0,0,1/4) 1/2,1/2,z  (4z,1,0,1/4)  
4. 4' (0,0,3/4) 1/2,-1/2,z  (4z,1,0,3/4)  

91.7.770 - 1 - 1532
**Generators selected**

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>(3) x,y,z+1/4 [v,u,w]</td>
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<tr>
<td></td>
<td>(4) y,x,z+3/4 [v,u,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>x,x,7/8 [u,u,w]</td>
<td>u,v,w</td>
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<tr>
<td></td>
<td>x,x,5/8 [u,u,w]</td>
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</tr>
<tr>
<td>8 b .2'</td>
<td>1/2,y,0 [u,0,w]</td>
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<td>1/2,1/2 [u,0,w]</td>
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<td>8 a .2</td>
<td>0,y,0 [0,v,0]</td>
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<td>0,y,1/2 [0,v,0]</td>
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<tr>
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<td>0,y,1/4 [v,0,0]</td>
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</table>

**Symmetry of Special Projections**

Along [0,0,1] p4'mmm'  
\( a^* = a \quad b^* = b \)

Along [1,0,0] p2mg'  
\( a^* = -c \quad b^* = b \)

Along [1,1,0] p2g* 2'mg'  
\( a^* = -c \quad b^* = (-a + b)/2 \)

Origin at 0,0,z  
Origin at x,0,1/4  
Origin at x,x,3/8
Origin on 2[1 1 0] at 2,1(1,2)

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

1. 1
   (1) 0,0,0
   (2) 0,0,1/2
   (3) 0,1/2,0
   (4) 1/2,0,0
   (5) 1/2,1/2,1/2
   (6) 1/2,1/2,1/4
   (7) 1/2,1/2,3/4
   (8) 1/2,1/2,3/4

2. 2
   (1) 0,0,1/2
   (2) 0,0,1/2
   (3) 0,0,1/2
   (4) 0,0,1/2

3. 4
   (1) 0,0,1/4
   (2) 0,0,1/4
   (3) 0,0,1/2
   (4) 0,0,1/4

4. 4
   (1) 1/2,1/2,1/2
   (2) 1/2,1/2,1/2
   (3) 1/2,1/2,1/4
   (4) 1/2,1/2,3/4

5. 4
   (1) 1/2,1/2,1/2
   (2) 1/2,1/2,1/2
   (3) 1/2,1/2,1/4
   (4) 1/2,1/2,3/4

6. 4
   (1) 1/2,1/2,1/2
   (2) 1/2,1/2,1/2
   (3) 1/2,1/2,1/4
   (4) 1/2,1/2,3/4
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y+1/2,x+1/2,z+3/4 [v,u,w]</td>
</tr>
<tr>
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<td>(5) x+1/2,y+1/2,z+1/4 [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z+3/4 [u,v,w]</td>
</tr>
<tr>
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<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
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</tbody>
</table>

4 a ..2      | x,x,0 [u,u,0]      |
|             | x,x,1/2 [u,u,0]    |
|             | x+1/2,x+1/2,1/4 [u,u,0] |
|             | x+1/2,x+1/2,3/4 [u,u,0] |

Symmetry of Special Projections

Along [0,0,1] p4g'm'            Along [1,0,0] p2g'g'            Along [1,1,0] p2'mg'
\( a^* = a \) \quad b^* = b \)   \( a^* = b \) \quad b^* = c \)   \( a^* = -c \) \quad b^* = (-a + b)/2
Origin at 0,1/2,z               Origin at x,1/4,3/8            Origin at x,x,0
Origin on 2 [1 1 0]1' at 2,1(1,2)1'

Asymmetric unit

\[0 \leq x < 1; \quad 0 \leq y < 1; \quad 0 \leq z < 1/8\]

Symmetry Operations

For 1 + set

(1) \(1\)
(1 | 0, 0, 0)

(5) \(2\) (0, 1/2, 0) \(1/4, y, 1/8\)
\((2, 1/2, 1/2, 1/4)\)

(6) \(2\) (1/2, 0, 0) \(x, 1/4, 3/8\)
\((2, 1/2, 1/2, 3/4)\)

(7) \(2\) \(x, x, 0\)
\((2, x, 0, 0, 0)\)

(8) \(2\) \(x, x, 1/4\)
\((2, x, 0, 0, 1/2)\)

For 1' + set

(1) \(1'\)
(1 | 0, 0, 0)'

(5) \(2'\) (0, 1/2, 0) \(1/4, y, 1/8\)
\((2, 1/2, 1/2, 1/4)'\)

(6) \(2'\) (1/2, 0, 0) \(x, 1/4, 3/8\)
\((2, 1/2, 1/2, 3/4)'\)

(7) \(2'\) \(x, x, 0\)
\((2, x, 0, 0, 0)'\)

(8) \(2'\) \(x, x, 1/4\)
\((2, x, 0, 0, 1/2)'\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>1 + 1'</td>
<td></td>
</tr>
<tr>
<td>8  b 11'</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z+1 [0,0,0]</td>
</tr>
<tr>
<td>(3) y+1/2,x+1/2,z+1/4 [0,0,0]</td>
<td>(4) y+1/2,x+1/2,z+1/4 [0,0,0]</td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z+1/4 [0,0,0]</td>
<td>(6) x+1/2,y+1/2,z+1/4 [0,0,0]</td>
</tr>
<tr>
<td>(7) y,x,z [0,0,0]</td>
<td>(8) y,x,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1'  
\[ a^* = a \quad b^* = b \]
Origin at 0,1/2,z

Along [1,0,0] p2gg1'  
\[ a^* = b \quad b^* = c \]
Origin at 1/4,3/8

Along [1,1,0] p2mg1'  
\[ a^* = -c \quad b^* = (-a + b)/2 \]
Origin at x,x,0
**Origin** on 2' [1 1 0] at 2,1(1,2')

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8 \]

**Symmetry Operations**

1. \( (1) 1 \)
   - \( (0,0,0) \)

2. \( (2) 2 \) \( (0,0,1/2) \) \( 0,0,z \)
   - \( (2_z \ 0,0,1/2) \)

3. \( (3) 4^{+} \) \( (0,0,1/4) \) \( 0,1/2,0 \)
   - \( (4_{z} \ 1/2,1/2,1/4) \)

4. \( (4) 4^{-} \) \( (0,0,3/4) \) \( 1/2,0,z \)
   - \( (4_{z}^{-} \ 1/2,1/2,3/4) \)

5. \( (5) 2 \) \( (0,1/2,0) \) \( 1/4,y,1/8 \)
   - \( (2_{y} \ 1/2,1/2,1/4) \)

6. \( (6) 2 \) \( (1/2,0,0) \) \( x,1/4,3/8 \)
   - \( (2_{x} \ 1/2,1/2,3/4) \)

7. \( (7) 2' \) \( x,x,0 \)
   - \( (2_{x} \ 0,0,0') \)

8. \( (8) 2' \) \( x,x,1/4 \)
   - \( (2_{x} \ 0,0,1/2') \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y+1/2,x+1/2,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z+3/4 [u,v,w]</td>
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<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>x,x,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x+1/2,1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x+1/2,3/4 [u,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'gm'  
Along [1,0,0] p2g'g'
Along [1,1,0] p2m'g'

a* = a  b* = b
Origin at 0,1/2,z

a* = b  b* = c
Origin at x,1/4,3/8

a* = -c  b* = (-a + b)/2
Origin at x,x,0
Origin on 2′ [1 1 0] at 2(1,1,2′)

Asymmetric unit

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8\]

Symmetry Operations

1. 1
   (1) 0,0,0
   (2) 2′ (0,0,1/2) 0,0,z
      (2′ z 0,0,1/2)
   (3) 4′ (0,0,1/4) 0,1/2,z
      (4′ z 1/2,1/2,1/4)
   (4) 4′ (0,0,3/4) 1/2,0,z
      (4′ z 1/2,1/2,3/4)

2. 2′ (0,1/2,0) 1/4,y,1/8
   (2′ z 1/2,1/2,1/4)

3. 2′ (1/2,0,0) x,1/4,3/8
   (2′ x 1/2,1/2,3/4)

4. 2′ x,x,0
   (2′ x 0,0,0)

5. 2′ (0,1/2,0) 1/4,y,1/8
   (2′ z 1/2,1/2,1/4)

6. 2′ (1/2,0,0) x,1/4,3/8
   (2′ x 1/2,1/2,3/4)

7. 2′ x,x,0
   (2′ x 0,0,0)

8. 2′ x,x,1/4
   (2′ x 0,0,1/2)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Positions</th>
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<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/4 [v,u,w]</td>
<td>(4) y+1/2,x+1/2,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/4 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+3/4 [u,v,w]</td>
</tr>
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<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x+1/2,1/4 [u,u,w]</td>
<td>x+1/2,x+1/2,3/4 [u,u,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p4gm
  - \( a^* = \mathbf{a} \quad b^* = \mathbf{b} \)
- **Along [1,0,0]**: p2'gg'
  - \( a^* = -\mathbf{c} \quad b^* = \mathbf{b} \)
- **Along [1,1,0]**: p2'mg'
  - \( a^* = -\mathbf{c} \quad b^* = (-\mathbf{a} + \mathbf{b})/2 \)

Origin at 0,1/2,z
Origin at x,1/4,3/8
Origin at x,x,0
P4,'2','2

92.5.775

P4,'2','2

Tetragonal

Origin on 2 [1 1 0] at 2,1(1,2)

Asymmetric unit

0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

(1) 1
(1) 0,0,0

(2) 2 (0,0,1/2) 0,0,z
(2z 0,0,1/2)

(3) 4+(0,0,1/4) 0,1/2,z
(4z 1/2,1/2,1/4)*

(4) 4- (0,0,3/4) 1/2,0,z
(4z-1)* 1/2,1/2,3/4)*

(5) 2'(0,1/2,0) 1/4,y,1/8
(2y 1/2,1/2,1/4)*

(6) 2' (1/2,0,0) x,1/4,3/8
(2x 1/2,1/2,3/4)*

(7) 2 x,x,0
(2xy 0,0,0)

(8) 2 x,x,1/4
(2xy 0,0,1/2)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{array}{cccc}
8 & b & 1 & (1) x,y,z [u,v,w] \\
 & & & (2) x,y,z+1/2 [u,v,w] \\
 & & & (3) y+1/2,x+1/2,z+1/4 [v,u,w] \\
 & & & (4) y+1/2,x+1/2,z+3/4 [v,u,w] \\
 & & & (5) x+1/2,y+1/2,z+1/4 [u,v,w] \\
 & & & (6) x+1/2,y+1/2,z+3/4 [u,v,w] \\
 & & & (7) y,x,z [v,u,w] \\
 & & & (8) y,x,z+1/2 [v,u,w] \\
4 & a & .2 & x,x,0 [u,u,0] \\
 & & & x,x,1/2 [u,u,0] \\
 & & & x+1/2,x+1/2,1/4 [u,u,0] \\
 & & & x+1/2,x+1/2,3/4 [u,u,0] \\
\end{array}
\]

Symmetry of Special Projections

Along [0,0,1] \quad p4'g'm \\
Along [1,0,0] \quad p2g'g' \\
Along [1,1,0] \quad p2m'g'

\[\begin{align*}
a^* &= a & b^* &= b \\
a^* &= b & b^* &= c \\
a^* &= -c & b^* &= (-a + b)/2 \\
\text{Origin at } 0,1/2,z & \quad \text{Origin at } x,1/4,3/8 & \quad \text{Origin at } x,x,0
\end{align*}\]
Origin at 222 at 421

Asymmetric unit  \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

1. \((1)\ 1 \quad (1\ 0,0,0)\)
2. \((2)\ 2\ 0,0,z \quad (2z\ 0,0,0)\)
3. \((3)\ 4^+\ (0,0,1/2)\ 0,0,z \quad (4z\ 0,0,1/2)\)
4. \((4)\ 4^-\ (0,0,1/2)\ 0,0,z \quad (4z^-1\ 0,0,1/2)\)
5. \((5)\ 2\ 0,y,0 \quad (2z\ 0,0,0)\)
6. \((6)\ 2\ x,0,0 \quad (2x\ 0,0,0)\)
7. \((7)\ 2\ x,x,1/4 \quad (2xy\ 0,0,1/2)\)
8. \((8)\ 2\ x,x,1/4 \quad (2xy\ 0,0,1/2)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 p 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x',y',z' [u',v',w']</td>
</tr>
<tr>
<td></td>
<td>(5) x',y',z' [u',v',w']</td>
<td>(3) y',x',z'+1/2 [v',u',w']</td>
</tr>
<tr>
<td></td>
<td>(7) y',x',z'+1/2 [v',u',w']</td>
<td>(8) y',x',z'+1/2 [v',u',w']</td>
</tr>
</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 o ...2</td>
<td>x,x,3/4 [u,u,0]</td>
<td>x',x,3/4 [u',u,0]</td>
</tr>
<tr>
<td></td>
<td>x',x,1/4 [u',u,0]</td>
<td>x',x,3/4 [u',u,0]</td>
</tr>
<tr>
<td>4 m ...2</td>
<td>x,1/2,0 [u,0,0]</td>
<td>1/2,x,1/2 [0,u,0]</td>
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<td>x',x,1/2 [u',0,0]</td>
<td>0,x,0 [0,u,0]</td>
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<td>4 l ...2</td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
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<td>x',0,1/2 [u',0,0]</td>
<td>0,x,0 [0,u,0]</td>
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<td>1/2,x,0 [0,u,0]</td>
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<td>x',1/2,1/2 [u',0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
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<td>4 j ...2</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
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<tr>
<td></td>
<td>x',0,0 [u',0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td>4 i ...2</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
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<tr>
<td>4 g ...2</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
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<td>0,0,0 [0,0,0]</td>
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<tr>
<td>2 f 2.22</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 e 2.22</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 d 222.</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 c 222.</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 222.</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>2 a 222.</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4m'm'

\[a^* = a \quad b^* = b\]

Origin at 0,0,z

Along [1,0,0] p2m'm'

\[a^* = b \quad b^* = c\]

Origin at x,0,0

Along [1,1,0] p2m'm'

\[a^* = (-a + b)/2 \quad b^* = c\]

Origin at x,x,1/4
Origin at 222 at 4z21

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4

Symmetry Operations

For 1 + set

1. \(1 (1 0,0,0)
2. \(2 0,0,z (2z 0,0,0)
3. \(4^* (0,0,1/2) 0,0,z (4z 0,0,1/2)
4. \(4^- (0,0,1/2) 0,0,z (4z^-1 0,0,1/2)
5. \(2 0,y,0 (2y 0,0,0)
6. \(2 x,0,0 (2x 0,0,0)
7. \(2 x,x,1/4 (2x 0,0,1/2)
8. \(2 x,x,1/4 (2x 0,0,1/2)

For 1' + set

1. \(1' (1 0,0,0)'
2. \(2' 0,0,z (2z 0,0,0)'
3. \(4'^* (0,0,1/2) 0,0,z (4z 0,0,1/2)'
4. \(4'^- (0,0,1/2) 0,0,z (4z^-1 0,0,1/2)'
5. \(2' 0,y,0 (2y 0,0,0)'
6. \(2' x,0,0 (2x 0,0,0)'
7. \(2' x,x,1/4 (2x 0,0,1/2)'
8. \(2' x,x,1/4 (2x 0,0,1/2)'

93.2.777 - 1 - 1546
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions
Multiplicity, 
Wyckoff letter, 
Site Symmetry.

<table>
<thead>
<tr>
<th>1 +</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 p 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z+1/2 [0,0,0]</td>
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<tr>
<td></td>
<td>(4) x,y,z+1/2 [0,0,0]</td>
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<tr>
<td></td>
<td>(5) x,y,z [0,0,0]</td>
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Symmetry of Special Projections
Along [0,0,1] p4mm1' 
Along [1,0,0] p2mm1' 
Along [1,1,0] p2mm1' 
\(a^* = a\) \(b^* = b\) 
\(a^* = b\) \(b^* = c\) 
\(a^* = (-a + b)/2\) \(b^* = c\) 
Origin at 0,0,z 
Origin at x,0,0 
Origin at x,x,1/4
Origin at 222 at 4'21

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

1. \( 1 \)
2. \( 0,0,z \)
3. \( 4^+ \cdot (0,0,1/2) \) \( 0,0,z \)
4. \( 4^- \cdot (0,0,1/2) \) \( 0,0,z \)
5. \( 0,y,0 \)
6. \( x,0,0 \)
7. \( 2^- \cdot x,x,1/4 \)
8. \( 2^+ \cdot x,x,1/4 \)

\( (1|0,0,0) \)
\( (2|0,0,0) \)
\( (4|0,0,1/2) \)
\( (4|0,0,1/2) \)
\( (2|0,0,0) \)
\( (2|x,0,0) \)
\( (2|x,0,0) \)
\( (2|x,0,0) \)

\( (2|0,0,0) \)
\( (2|x,0,0) \)
\( (2|x,0,0) \)
Continued 93.3.778 P4_{22'}

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
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<tr>
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<td>(3) y,x,z+1/2 [v,u,w]</td>
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<td>x,x,3/4 [u,u,w]</td>
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<td>1/2,x,1/2 [0,u,0]</td>
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<td>x,0,0 [u,0,0]</td>
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<td>1/2,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>0,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>1/2,1/2,3/4 [0,0,w]</td>
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<tr>
<td>2 e 2.2'2'</td>
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<td>0,0,3/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
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<td>1/2,0,0 [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1] p4'mm'  
Along [1,0,0] p2m'm'  
Along [1,1,0] p2'm'm'

\[
a^* = a \quad b^* = b \\
\text{Origin at 0,0,0}
\]

\[
a^* = b \quad b^* = c \\
\text{Origin at x,0,0}
\]

\[
a^* = -c \quad b^* = (-a + b)/2 \\
\text{Origin at x,x,1/4}
\]
Origin at 22'2' at 42'2'1

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4\)

Symmetry Operations

1. \(1\), \(0,0,0\)
2. \(2\), \(0,0,z\)
3. \(2'\), \(0,0,1/2\)
4. \(4'\), \(0,0,0\)
5. \(2'\), \(0,y,0\)
6. \(2'\), \(0,0,0\)
7. \(2'\), \(x,0,1/4\)
8. \(2'\), \(x,0,0\)

\(2'\), \(y,0,0\)
\(2'\), \(0,0,0\)
\(2'\), \(x,x,1/4\)
\(2'\), \(0,0,1/2\)
Continued 93.4.779  P4₂₂'²

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(3) x,y,z+1/2 [v,u,w]</td>
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Symmetry of Special Projections

Along [0,0,1]  p4mm
a⁺ = a  b⁺ = b
Origin at 0,0,z

Along [1,0,0]  p2'mm'
a⁺ = -c  b⁺ = b
Origin at x,0,0

Along [1,1,0]  p2'mm'
a⁺ = -c  b⁺ = (-a + b)/2
Origin at x,x,1/4

93.4.779 - 2 - 1551
Origin at 2\(\overline{2}\)\(\overline{2}\) at 4\(\overline{2}\)\(\overline{2}\)

Asymmetric unit: 
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4\]

Symmetry Operations:

1. \((1)\) \(1\)
   
   \(1\) \(0,0,0)\)

2. \((2)\) \(2\)
   
   \(2\) \(0,0,z\)
   
   \(2\) \(0,0,0)\)

3. \((3)\) \(4^+\)
   
   \(4^+\) \((0,0,1/2)\)
   
   \(4^+\) \(0,0,1/2)\)

4. \((4)\) \(4^-\)
   
   \(4^-\) \((0,0,1/2)\)
   
   \(4^-\) \(0,0,1/2)\)

5. \((5)\) \(2'\)
   
   \(2'\) \(0,y,0\)
   
   \(2'\) \(0,0,0)\)

6. \((6)\) \(2'\)
   
   \(2'\) \(x,0,0\)
   
   \(2'\) \(0,0,0)\)

7. \((7)\) \(2\)
   
   \(2\) \(x,x,1/4\)
   
   \(2\) \(0,0,1/2)\)

8. \((8)\) \(2\)
   
   \(2\) \(x,x,1/4\)
   
   \(2\) \(0,0,1/2)\)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

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**Symmetry of Special Projections**

Along [0,0,1] p4'm'm' Along [1,0,0] p2'm'm' Along [1,1,0] p2m'm'

\[ a^* = a \] \[ b^* = b \] \[ a^* = -c \] \[ b^* = b \] \[ a^* = (-a + b)/2 \] \[ b^* = c \]

Origin at 0,0,z Origin at x,0,0 Origin at x,x,1/4
Origin at 2'22' at 4_2(22')1

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4\]

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
   \[(1)\ (0,0,0)\]
2. \(2'\)
   \[(2)\ 0,0,z\]
   \[(2z_1)\ 0,0,0)\]
3. \(4^*\)
   \[(3)\ (0,0,1/2)\ 0,0,z\]
   \[
   (4z_1)\ 0,0,1/2)\]
4. \(4^-\)
   \[(4)\ (0,0,1/2)\ 0,0,z\]
   \[
   (4z_1)\ 0,0,1/2)\]
5. \(2'\)
   \[(5)\ 0,y,0\]
   \[(2z_1)\ 0,0,0)\]
6. \(2\)
   \[(6)\ x,0,0\]
   \[
   (2z_1)\ 0,0,0)\]
7. \(2\)
   \[(7)\ x,x,1/4\]
   \[
   (2xy)\ 0,0,1/2)\]
8. \(2'\)
   \[(8)\ x,x,1/4\]
   \[
   (2xy)\ 0,0,1/2)\]

For \((0,0,1)\) + set

1. \(t'\)
   \[(1)\ (0,0,1)\]
   \[(1)\ 0,0,1)\]
2. \(2\)
   \[(2)\ (0,0,1)\ 0,0,z\]
   \[
   (2z_1)\ 0,0,1)\]
3. \(4^*\)
   \[(3)\ (0,0,3/2)\ 0,0,z\]
   \[
   (4z_1)\ 0,0,3/2)\]
4. \(4^-\)
   \[(4)\ (0,0,3/2)\ 0,0,z\]
   \[
   (4z_1)\ 0,0,3/2)\]
5. \(2\)
   \[(5)\ 0,y,1/2\]
   \[
   (2z_1)\ 0,0,1)\]
6. \(2'\)
   \[(6)\ x,0,1/2\]
   \[
   (2z_1)\ 0,0,1)\]
7. \(2'\)
   \[(7)\ x,x,3/4\]
   \[
   (2xy)\ 0,0,3/2)\]
8. \(2\)
   \[(8)\ x,x,3/4\]
   \[
   (2xy)\ 0,0,3/2)\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Continued

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tr>
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<td>x,x,3/4 [u,u,w]</td>
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<td>4 g</td>
<td>0,0,0 [v,u,0]</td>
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<tr>
<td>4 f</td>
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</table>

Symmetry of Special Projections

Along [0,0,1]  p4mm1'  
Along [1,0,0]  p2a'2mm  
Along [1,1,0]  p2a'2mm

a* = a  b* = b  
a* = -c  b* = b  
a* = -c  b* = (-a + b)/2

Origin at 0,0,0  
Origin at x,0,0  
Origin at x,x,1/4
Origin at 222 at 4\textsubscript{2}1

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1
(1) 0,0,0

(2) 1 0,0,z
(2\textsubscript{x} 0,0,0)

(3) 4\textsuperscript{*} (0,0,1/2) 0,0,z
(4\textsubscript{x} 0,0,1/2)

(4) 4\textsuperscript{*} (0,0,1/2) 0,0,z
(4\textsubscript{x} 0,0,1/2)

For $(1,0,0)' + set

(1) t' (1,0,0)
(1) 1,0,0)

(2) 2' 1/2,0,z
(2\textsubscript{x} 1,0,0)

(3) 4\textsuperscript{*}' (0,0,1/2) 1/2,1/2,z
(4\textsubscript{x} 1,0,1/2)

(4) 4\textsuperscript{*}' (0,0,1/2) 1/2,-1/2,z
(4\textsubscript{x} 1,0,1/2)

For $(1,0,0)' + set

(1) t' (1,0,0)
(1) 1,0,0)

(2) 2' 1/2,0,z
(2\textsubscript{x} 1,0,0)

(3) 4\textsuperscript{*}' (0,0,1/2) 1/2,1/2,z
(4\textsubscript{x} 1,0,1/2)

(4) 4\textsuperscript{*}' (0,0,1/2) 1/2,-1/2,z
(4\textsubscript{x} 1,0,1/2)
Generators selected  (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>x,x,3/4 [u,u,0]</td>
<td>x',x,1/4 [u',u,0]</td>
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<td>x,x,1/4 [u,u,0]</td>
<td>x',x,3/4 [u',u,0]</td>
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<td>x,1/2,0 [0,v,w]</td>
<td>x',1/2,1/2 [0,v,w]</td>
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<td>8 l</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x',0,1/2 [u,0,0]</td>
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<tr>
<td>8 k</td>
<td>x,1/2,1/2 [0,v,w]</td>
<td>x',1/2,1/2 [0,v,w]</td>
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<td>x',0,0 [u,0,0]</td>
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<td>0,1/2,z [u,v,0]</td>
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<td>8 h</td>
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<td>8 g</td>
<td>0,0,z [0,0,0]</td>
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<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] \( p_0 \): 4m'm'
  \( a^* = a \quad b^* = b \)
  Origin at 0,0,z

- Along [1,0,0] \( p_{2mm} \): 1'1'
  \( a^* = b \quad b^* = c \)
  Origin at x,0,0

- Along [1,1,0] \( p_{2a} \): 2m'm'
  \( a^* = (-a + b)/2 \quad b^* = c \)
  Origin at x,x,1/4

93.7.782 - 2 - 1557
Origin at 2'22' at 42 (2,2')1

Asymmetric unit 
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

For (0,0,0) + set

(1) \( \mathbf{1} \)
(1) \( (0,0,0) \)
(2) \( 2' \; 0,0,z \)
(2) \( (2z,0,0) \)
(3) \( 4' \; (0,0,1/2) \; 0,0,z \)
(3) \( (4z,0,0,1/2) \)
(4) \( 4' \; (0,0,1/2) \; 0,0,z \)
(4) \( (4z,0,0,1/2) \)

For (1,0,0)' + set

(1) \( t' \; (1,0,0) \)
(1) \( (1,0,0)' \)
(2) \( 2 \; 1/2,0,z \)
(2) \( (2z,1,0,0) \)
(3) \( 4' \; (0,0,1/2) \; 1/2,1/2,z \)
(3) \( (4z,1,0,1/2) \)
(4) \( 4' \; (0,0,1/2) \; 1/2,-1/2,z \)
(4) \( (4z,1,0,1/2) \)

Generators selected

(1); \( t'(1,0,0) \); \( t'(0,1,0) \); \( t'(0,0,1) \); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[ (0,0,0) + \quad (1,0,0)' + \]

\[ 16 \quad p \quad 1 \]

(1) \( x,y,z \; [u,v,w] \)
(2) \( x,y,z \; [u,v,w] \)
(3) \( y,x,z+1/2 \; [v,u,w] \)
(4) \( y,x,z+1/2 \; [v,u,w] \)

(5) \( x,y,z \quad [u,v,w] \)
(6) \( x,y,z \quad [u,v,w] \)
(7) \( y,x,z+1/2 \; [v,u,w] \)
(8) \( y,x,z+1/2 \; [v,u,w] \)

\[ 8 \quad o \quad .2' \]

(1) \( x,x,3/4 \; [u,u,w] \)
(2) \( x,x,3/4 \; [u,u,w] \)
(3) \( x,x,3/4 \; [v,u,w] \)
(4) \( x,x,3/4 \; [v,u,w] \)

\[ 8 \quad n \quad .2 \]

(1) \( x,x,1/4 \; [u,u,0] \)
(2) \( x,x,1/4 \; [u,u,0] \)
(3) \( x,x,1/4 \; [v,u,0] \)
(4) \( x,x,1/4 \; [v,u,0] \)

\[ 8 \quad m \quad .2' \]

(1) \( x,1/2,0 \; [0,v,w] \)
(2) \( x,1/2,0 \; [0,v,w] \)
(3) \( x,1/2,0 \; [0,v,w] \)
(4) \( x,1/2,0 \; [0,v,w] \)

\[ 8 \quad l \quad .2' \]

(1) \( x,0,1/2 \; [0,v,w] \)
(2) \( x,0,1/2 \; [0,v,w] \)
(3) \( x,0,1/2 \; [0,v,w] \)
(4) \( x,0,1/2 \; [0,v,w] \)

\[ 8 \quad k \quad .2 \]

(1) \( x,1/2,1/2 \; [u,0,0] \)
(2) \( x,1/2,1/2 \; [u,0,0] \)
(3) \( x,1/2,1/2 \; [u,0,0] \)
(4) \( x,1/2,1/2 \; [u,0,0] \)

\[ 8 \quad j \quad .2 \]

(1) \( x,0,0 \; [u,0,0] \)
(2) \( x,0,0 \; [u,0,0] \)
(3) \( x,0,0 \; [u,0,0] \)
(4) \( x,0,0 \; [u,0,0] \)

\[ 8 \quad i \quad .2' \]

(1) \( 0,1/2,z \; [0,0,w] \)
(2) \( 0,1/2,z \; [0,0,w] \)
(3) \( 0,1/2,z \; [0,0,w] \)
(4) \( 0,1/2,z \; [0,0,w] \)

\[ 8 \quad h \quad .2' \]

(1) \( 1/2,1/2,z \; [v,u,0] \)
(2) \( 1/2,1/2,z \; [v,u,0] \)
(3) \( 1/2,1/2,z \; [v,u,0] \)
(4) \( 1/2,1/2,z \; [v,u,0] \)

\[ 8 \quad g \quad .2' \]

(1) \( 0,0,z \; [u,v,0] \)
(2) \( 0,0,z \; [u,v,0] \)
(3) \( 0,0,z \; [u,v,0] \)
(4) \( 0,0,z \; [u,v,0] \)

\[ 4 \quad f \quad .2',22' \]

(1) \( 1/2,1,2,1/4 \; [u,u,0] \)
(2) \( 1/2,1,2,1/4 \; [u,u,0] \)
(3) \( 1/2,1,2,1/4 \; [u,u,0] \)
(4) \( 1/2,1,2,3/4 \; [u,u,0] \)

\[ 4 \quad e \quad .2',22' \]

(1) \( 0,0,1/4 \; [u,u,0] \)
(2) \( 0,0,1/4 \; [u,u,0] \)
(3) \( 0,0,1/4 \; [u,u,0] \)
(4) \( 0,0,1/4 \; [u,u,0] \)
Symmetry of Special Projections

Along [0,0,1] p4mm1’
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2mm1’
\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,0,0

Along [1,1,0] p\_\infty 2mm
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,1/4
Origin at 2'22' at 42'21

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

For (0,0,0) + set

1. \( \{1\} \)
2. \( \{2'\} 0,0,z \) \( (2_z|0,0,0)' \)
3. \( \{4'\} (0,0,1/2) 0,0,z \) \( (4_z|0,0,1/2)' \)
4. \( \{4'\} (0,0,1/2) 0,0,z \) \( (4_z^{-1}|0,0,1/2) \)
5. \( \{2'\} 0,y,0 \) \( (2_y|0,0,0)' \)
6. \( \{2\} x,0,0 \) \( (2_x|0,0,0) \)
7. \( \{2'\} x,x,1/4 \) \( (2_{xy}|0,0,1/2)' \)
8. \( \{2\} x,x,1/4 \) \( (2_{xy}|0,0,1/2) \)

For (0,0,1) + set

1. \( \{t'\} (0,0,1) \)
2. \( \{2\} (0,0,1) 0,0,z \) \( (2_z|0,0,1) \)
3. \( \{4'\} (0,0,3/2) 0,0,z \) \( (4_z|0,0,3/2) \)
4. \( \{4'\} (0,0,3/2) 0,0,z \) \( (4_z^{-1}|0,0,3/2)' \)
5. \( \{2\} 0,y,1/2 \) \( (2_y|0,0,1) \)
6. \( \{2'\} x,0,1/2 \) \( (2_x|0,0,1)' \)
7. \( \{2\} x,x,3/4 \) \( (2_{xy}|0,0,3/2) \)
8. \( \{2'\} x,x,3/4 \) \( (2_{xy}|0,0,3/2)' \)
Generators selected: (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td></td>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
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</tr>
<tr>
<td>8 o</td>
<td>.2</td>
<td>x,x,3/4 [u,u,0]</td>
<td>x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td>8 n</td>
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<td>x,x,1/4 [u,u,w]</td>
<td>x,x,3/4 [u,u,w]</td>
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<tr>
<td>8 m</td>
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<td>1/2,x,1/2 [0,u,0]</td>
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<td>x,0,1/2 [0,v,w]</td>
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<td>x,1/2,1/2 [0,v,w]</td>
<td>1/2,x,0 [v,0,w]</td>
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<td>8 j</td>
<td>.2</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>.2'</td>
<td>0,1/2,z [u,v,0]</td>
<td>1/2,0,z+1/2 [v,u,0]</td>
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<td>8 h</td>
<td>.2'</td>
<td>1/2,1/2,z [u,v,0]</td>
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<td>8 g</td>
<td>.2'</td>
<td>0,0,z [u,v,0]</td>
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<td>4 f</td>
<td>2',2'</td>
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<td>0,1/2,1/2 [0,v,0]</td>
<td>1/2,0,0 [v,0,0]</td>
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<td>1/2,0,1/2 [0,u,0]</td>
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<td>2',2'</td>
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<td>2',2'</td>
<td>0,0,0 [u,0,0]</td>
<td>0,0,1/2 [0,u,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm1'

a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2a* 2mm

a* = -c  b* = b
Origin at x,0,0

Along [1,1,0] p2a* 2mm

a* = -c  b* = (-a + b)/2
Origin at x,x,3/4
**Origin** at 222 at 4'21

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

For \((0,0,0) + \) set

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<tr>
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<th>Operation</th>
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<tr>
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<td>(0,0,z)</td>
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<tr>
<td>(2) 2</td>
<td>((2_z,0,0,0))</td>
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<tr>
<td>(3) 4'</td>
<td>((0,0,1/2),0,0,z)</td>
</tr>
<tr>
<td>(4) 4'</td>
<td>((0,0,1/2),0,0,z)</td>
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For \((1,0,0)' + \) set

<table>
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<tr>
<td>(1) t'</td>
<td>((1,1,0,0))</td>
</tr>
<tr>
<td>(2) 2'</td>
<td>(1/2,0,0)</td>
</tr>
<tr>
<td>(2) 2'</td>
<td>((2_z,1,0,0))</td>
</tr>
<tr>
<td>(3) 4'</td>
<td>((0,0,1/2),1/2,1/2,z)</td>
</tr>
<tr>
<td>(4) 4'</td>
<td>((0,0,1/2),1/2,1/2,z)</td>
</tr>
</tbody>
</table>

The diagram illustrates the Crystal System P\(\_p\) 4'22' with unit cell parameters and symmetry operations. The asymmetric unit and origin are marked, and the symmetry operations are listed for both \((0,0,0)\) and \((1,0,0)\) sets.
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinantes

\[(0,0,0) + \ (1,0,0)'+ \]

\[
\begin{array}{cccc}
16 & p & 1 & (1) \ x,y,z \ [u,v,w] \\
 & & & (2) \bar{x},y,z \ [\bar{u},v,w] \\
 & & & (3) \ y,x,z+1/2 \ [v,\bar{u},\bar{w}] \\
 & & & (4) \ y,x,z+1/2 \ [v,\bar{u},\bar{w}] \\
 & & & (5) \bar{x},y,z \ [\bar{u},v,w] \\
8 & o & ..2' & x,x,3/4 \ [u,\bar{u},w] \\
 & & & \bar{x},\bar{x},3/4 \ [\bar{u},u,w] \\
8 & n & ..2' & x,x,1/4 \ [u,\bar{u},w] \\
 & & & \bar{x},\bar{x},1/4 \ [\bar{u},u,w] \\
8 & m & .2' & x,1/2,0 \ [0,v,w] \\
 & & & \bar{x},1/2,0 \ [\bar{v},u,w] \\
8 & l & .2 & x,0,1/2 \ [u,0,0] \\
 & & & \bar{x},0,1/2 \ [\bar{u},0,0] \\
8 & k & .2' & x,1/2,1/2 \ [0,v,w] \\
 & & & \bar{x},1/2,1/2 \ [\bar{v},0,w] \\
8 & j & .2 & x,0,0 \ [u,0,0] \\
 & & & \bar{x},0,0 \ [\bar{u},0,0] \\
8 & i & ..2' & 0,1/2,z \ [u,v,0] \\
 & & & 1/2,0,z+1/2 \ [\bar{v},0,w] \\
8 & h & .2 & 1/2,1/2,z \ [0,0,w] \\
 & & & 1/2,1/2,z \ [0,0,w] \\
8 & g & .2 & 0,0,z \ [0,0,w] \\
 & & & 0,z+1/2 \ [0,0,w] \\
4 & f & 2.2' & 1/2,1/2,1/4 \ [0,0,w] \\
 & & & 1/2,1/2,3/4 \ [0,0,w] \\
4 & e & 2.2' & 0,0,1/4 \ [0,0,w] \\
 & & & 0,3/4 \ [0,0,w] \\
4 & d & 22' & 0,1/2,1/2 \ [0,v,0] \\
 & & & 1/2,0,0 \ [\bar{v},0,w] \\
4 & c & 22' & 0,1/2,0 \ [0,v,0] \\
 & & & 1/2,0,1/2 \ [\bar{v},0,w] \\
4 & b & 22' & 1/2,1/2,0 \ [0,0,w] \\
 & & & 1/2,1/2,1/2 \ [0,0,w] \\
4 & a & 222 & 0,0,0 \ [0,0,0] \\
 & & & 0,1/2 \ [0,0,0] \\
\end{array}
\]

Symmetry of Special Projections

Along [0,0,1] \( p_r \), 4mm
\( a^* = a \ \ b^* = b \)
Origin at 1/2,1/2,z

Along [1,0,0] \( p2mm1' \)
\( a^* = b \ \ b^* = c \)
Origin at x,0,0

Along [1,1,0] \( p_{2e} \), 2mm
\( a^* = (-a + b)/2 \ \ b^* = c \)
Origin at x-1/4,x+1/4,1/4
P4₂ 2₁ 2₁
94.1.786

P4₂ 2₁ 2₁
422

Tetragonal

Origin on 222 at 212

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2
\]

Symmetry Operations

(1) 1
(2) 2 0,0,0
(3) 4⁺ (0,0,1/2) 0,1/2,z
(4) 4⁻ (0,0,1/2 1/2,0,z

(5) 2 (0,1/2,0) 1/4,y,1/4
(2₁ 1/2,1/2,1/2)
(6) 2 (1/2,0,0) x,1/4,1/4
(2₁ 1/2,1/2,1/2)
(7) 2 x,x,0
(2ₓ 0,0,0)
(8) 2 x,0,0
(2ₓ 0,0,0)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w] (4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w] (6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w] (8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 f .2</td>
<td>x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x+1/2,x+1/2,0 [u,u,0] x+1/2,x+1/2,0 [u,u,0]</td>
</tr>
<tr>
<td>4 e .2</td>
<td>x,x,0 [u,u,0] x,x,0 [u,u,0] x+1/2,x+1/2,1/2 [u,u,0] x+1/2,x+1/2,1/2 [u,u,0]</td>
</tr>
<tr>
<td>4 d 2..</td>
<td>0,1/2,z [0,0,w] 0,1/2,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 c 2..</td>
<td>0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 b 2.22</td>
<td>0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 2.22</td>
<td>0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4g'm'  
Along [1,0,0] p2m'g'  
Along [1,1,0] p2m'm'

\[ \mathbf{a}^* = \mathbf{a} \]  
\[ \mathbf{b}^* = \mathbf{b} \]  
\[ \mathbf{a}^* = \mathbf{b} \]  
\[ \mathbf{b}^* = \mathbf{c} \]  
\[ \mathbf{a}^* = \mathbf{a} + \mathbf{b} \]  
\[ \mathbf{b}^* = \mathbf{c} \]  
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \]  
\[ \mathbf{b}^* = \mathbf{c} \]

Origin at 0,1/2,z  
Origin at x,1/4,1/4  
Origin at x,x,0
**Origin** on $2221'$ at $2121'$

**Asymmetric unit** $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$

**Symmetry Operations**

For 1 + set

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) $0,0,0$

(3) 4' (0,0,1/2) 0,1/2,z
(4) $4,1/2,1/2,1/2,1/2$

(4) $4,1/2,1/2,1/2,1/2$

For 1' + set

(1) 1'
(1) 0,0,0'

(2) 2' 0,0,z
(2) $0,0,0'$

(3) 4'' (0,0,1/2) 0,1/2,z
(4) $4,1/2,1/2,1/2,1/2$

(4) $4,1/2,1/2,1/2,1/2$

(5) 2' (0,1/2,0) 1/4,y,1/4
(5) $1/2,1/2,1/2$

(6) 2' (1/2,0,0) x,1/4,1/4
(6) $2x,1/2,1/2,1/2$

(7) 2' x,x,0
(7) $2x,0,0,0$

(8) 2' x,x,0
(8) $2x,0,0,0$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(3) y+1/2,x+1/2,z+1/2 [0,0,0] (4) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z+1/2 [0,0,0] (6) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(7) y,x,z [0,0,0] (8) y,x,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 f .21' x,x,1/2 [0,0,0] x,x,1/2 [0,0,0] x+1/2,x+1/2,0 [0,0,0] x+1/2,x+1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 e .21' x,x,0 [0,0,0] x,x,0 [0,0,0] x+1/2,x+1/2,1/2 [0,0,0] x+1/2,x+1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 d 2.1' 0,1/2,z [0,0,0] 0,1/2,z+1/2 [0,0,0] 1/2,0,z+1/2 [0,0,0] 1/2,0,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 c 2.1' 0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 0,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b 2.221' 0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 2.221' 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Origin at 0,1/2,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p4gm1' a* = a b* = b</td>
</tr>
<tr>
<td>Along [1,0,0] p2mg1' a* = b b* = c</td>
</tr>
<tr>
<td>Along [1,1,0] p2mm1' a* = (-a + b)/2 b* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
</tr>
<tr>
<td>Along [1,0,0] p2mg1' a* = b b* = c</td>
</tr>
<tr>
<td>Along [1,1,0] p2mm1' a* = (-a + b)/2 b* = c</td>
</tr>
<tr>
<td>Origin at x,1/4,1/4</td>
</tr>
<tr>
<td>Along [1,0,0] p2mg1' a* = b b* = c</td>
</tr>
<tr>
<td>Along [1,1,0] p2mm1' a* = (-a + b)/2 b* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 22'2' at 212'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
   (1) 0,0,0
(2) 2 0,0,z
   (2) z 0,0,0
(3) 4+ ' (0,0,1/2) 0,1/2,z
   (3z) 1/2,1/2,1/2
(4) 4- ' (0,0,1/2) 1/2,0,z
   (4z) -1 1/2,1/2,1/2
(5) 2 (0,1/2,0) 1/4,y,1/4
   (5z) 1/2,1/2,1/2
(6) 2 (1/2,0,0) x,1/4,1/4
   (6z) 1/2,1/2,1/2
(7) 2' x,x,0
   (7z) 0,0,0
(8) 2' x,x,0
   (8z) 0,0,0

P4₁'2', 2'

94.3.788

P4₁'2', 2'

Tetragonal
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w] (4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w] (6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w] (8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 f ..2'</td>
<td>x,x,1/2 [u,u,w] x,x,1/2 [u,u,w] x+1/2,x+1/2,0 [u,u,w] x+1/2,x+1/2,0 [u,u,w]</td>
</tr>
<tr>
<td>4 e ..2'</td>
<td>x,x,0 [u,u,w] x,x,0 [u,u,w] x+1/2,x+1/2,1/2 [u,u,w] x+1/2,x+1/2,1/2 [u,u,w]</td>
</tr>
<tr>
<td>4 d 2'</td>
<td>0,1/2,z [0,0,w] 0,1/2,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 c 2'</td>
<td>0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 b 2.2'</td>
<td>0,0,1/2 [0,0,w] 1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 a 2.2'</td>
<td>0,0,0 [0,0,w] 1/2,1/2,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]** p4g'm'
  - \( a^* = a \) \( b^* = b \)
  - Origin at 0,1/2,z

- **Along [1,0,0]** p2m'g'
  - \( a^* = b \) \( b^* = c \)
  - Origin at x,1/4,1/4

- **Along [1,1,0]** p2'mm'
  - \( a^* = -c \) \( b^* = (-a + b)/2 \)
  - Origin at x,x,0
**Origin** on 22'2' at 212'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

1. \( 1 \)
   
   \[
   (1) \begin{cases}
   0,0,0 \\
   (1,0,0,0)
   \end{cases}
   \]

2. \( 2 \)
   
   \[
   (2) 2 \quad (0,0,z) \\
   (2_x 0,0,0)
   \]

3. \( 4' \)
   
   \[
   (3) 4' (0,0,1/2) \quad 0,1/2,z \\
   (4_z 1/2,1/2,1/2)
   \]

4. \( 4' \)
   
   \[
   (4) 4' (0,0,1/2) \quad 1/2,0,z \\
   (4_z^{-1} 1/2,1/2,1/2)
   \]

5. \( 2' \)
   
   \[
   (5) 2' (0,1/2,0) \quad 1/4,y,1/4 \\
   (2_y 1/2,1/2,1/2)
   \]

6. \( 2' \)
   
   \[
   (6) 2' (1/2,0,0) \quad x,1/4,1/4 \\
   (2_x 1/2,1/2,1/2)
   \]

7. \( 2' \)
   
   \[
   (7) 2' x,x,0 \\
   (2_x 0,0,0)
   \]

8. \( 2' \)
   
   \[
   (8) 2' x,x,0 \\
   (2_x 0,0,0)
   \]

\[ 94.4.789 - 1 - 1571 \]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 f ..2'</td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
<td>x+1/2,x+1/2,0 [u,u,w]</td>
</tr>
<tr>
<td>4 e ..2'</td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
<td>x+1/2,x+1/2,1/2 [u,u,w]</td>
</tr>
<tr>
<td>4 d .2'</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 2.2'2'</td>
<td>0,0,1/2 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 a 2.2'2'</td>
<td>0,0,0 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm  | Along [1,0,0] p2'mg'  | Along [1,1,0] p2'mm'
\(a^* = a\) \(b^* = b\)  | \(a^* = b\) \(b^* = c\)  | \(a^* = -c\) \(b^* = (-a + b)/2\)
Origin at 0,1/2,z  | Origin at x,1/4,1/4  | Origin at x,x,0
Origin on 222 at 212

Asymmetric unit \(0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2\)

Symmetry Operations

1. \(1\)  
   \(1|0,0,0\)

2. \(2\)  
   \(0,0,z\)  
   \(2_z|0,0,0\)

3. \(4^+\)  
   \((0,0,1/2)\)  
   \(0,1/2,z\)  
   \(4_z |1/2,1/2,1/2\)

4. \(4^-\)  
   \((0,0,1/2)\)  
   \(1/2,0,z\)  
   \(4_z^- |1/2,1/2,1/2\)

5. \(2^+\)  
   \((0,1/2,0)\)  
   \(1/4,y,1/4\)  
   \((2_y |1/2,1/2,1/2)\)

6. \(2^-\)  
   \((1/2,0,0)\)  
   \(x,1/4,1/4\)  
   \((2_x |1/2,1/2,1/2)\)

7. \(2\)  
   \(x,x,0\)  
   \((2_{xy} |0,0,0)\)

8. \(2\)  
   \(x,x,0\)  
   \((2_{xy} |0,0,0)\)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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<td>x,x,1/2 [u,u,0]</td>
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<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
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<td>1/2,0,z+1/2 [0,0,w]</td>
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<tr>
<td>4 c 2..</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
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<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2 a 2.22</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p4g'm'
  \[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]
- Along [1,0,0] p2m'g'
  \[ \mathbf{a}^* = \mathbf{b}, \quad \mathbf{b}^* = \mathbf{c} \]
- Along [1,1,0] p2m'm'
  \[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2, \quad \mathbf{b}^* = \mathbf{c} \]

Origin at 0,1/2,z  
Origin at x,1/4,1/4  
Origin at x,x,0
**Origin** on 2'22 at 2'12

**Asymmetric unit**  
0 ≤ x ≤ 1/2;  0 ≤ y ≤ 1/2;  0 ≤ z ≤ 1/2

**Symmetry Operations**

For (0,0,0) + set:

1. \(1\)
   
2. \(2'\) 0,0,z  
   \((2_z 0,0,0)\)

3. \(4^*\) (0,0,1/2) 0,1/2,z  
   \((4_z 1/2,1/2,1/2)\)

4. \(4^{-1}\) (0,0,1/2) 1/2,0,z  
   \((4_z^{-1} 1/2,1/2,1/2)\)

For (0,0,1') + set:

1. \(t'\) (0,0,1)  
   \((1 0,0,1)\)

2. \(2\) (0,0,1) 0,0,z  
   \((2_z 0,0,1)\)

3. \(4^*\) (0,0,3/2) 0,1/2,z  
   \((4_z 1/2,1/2,3/2)\)

4. \(4^{-1}\) (0,0,3/2) 1/2,0,z  
   \((4_z^{-1} 1/2,1/2,3/2)\)

For (0,1,0) + set:

5. \(2\) (0,1/2,0) 1/4,y,1/4  
   \((2_y 1/2,1/2,1/2)\)

6. \(2'\) (1/2,0,0) x,1/4,1/4  
   \((2_x 1/2,1/2,1/2)\)

7. \(2'\) x,x,0  
   \((2_{xy} 0,0,0)\)

8. \(2\) x,x,0  
   \((2_{xy} 0,0,0)\)

9. \(94.6.791 - 1 - 1575\)
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

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<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>16 g 1</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>16 g 2</td>
<td>16 g 3</td>
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<tr>
<td>16 g 4</td>
<td>16 g 5</td>
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<td>16 g 6</td>
<td>16 g 7</td>
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<tr>
<td>16 g 8</td>
<td>16 g 9</td>
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</table>

| 8 f ..2      | x,x,1/2 [u,u,0] |
| 8 e ..2'     | x,x,0 [u,u,0]  |
| 8 d 2'       | 1/2,0,z+1/2 [v,u,0] |
| 8 c 2'       | 1/2,1/2,z+1/2 [v,u,0] |
| 4 b 2'2'     | 0,0,1/2 [u,u,0] |
| 4 a 2'2'2    | 0,0,0 [u,u,0]  |

Symmetry of Special Projections

Along [0,0,1] \( \text{p4gm1'} \)  
\( a^* = a \quad b^* = b \)  
Origin at 0,1/2,z

Along [1,0,0] \( \text{p}_{2a} \) \( \text{2mg} \)  
\( a^* = b \quad b^* = c \)  
Origin at x,1/4,1/4

Along [1,1,0] \( \text{p}_{2a} \) \( \text{2mm} \)  
\( a^* = -c \quad b^* = (-a + b)/2 \)  
Origin at x,x,1/2
**Origin** on $2'2'2'$ at $2(1,2')(2',1)$

**Asymmetric unit**

\[0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2\]

**Symmetry Operations**

For $(0,0,0)$ + set

1. $1$
   - \[(0,0,0)\]

2. $2' \ 0,0,z$
   - \[(2_z,0,0,0)\]

3. $4^+ \ (0,0,1/2) \ 0,1/2,z$
   - \[(4_z|1/2,1/2,1/2)'\]

4. $4^- \ (0,0,1/2) \ 1/2,0,z$
   - \[(4_z^{-1}|1/2,1/2,1/2)\]

For $(0,0,1)'$ + set

1. $t' \ (0,0,1)$
   - \[(1,0,0,1)\]

2. $2 \ (0,0,1) \ 0,0,z$
   - \[(2_z,0,0,1)\]

3. $4^+ \ (0,0,3/2) \ 0,1/2,z$
   - \[(4_z|1/2,1/2,3/2)\]

4. $4^- \ (0,0,3/2) \ 1/2,0,z$
   - \[(4_z^{-1}|1/2,1/2,3/2)'\]

For $(0,1,1)$ + set

5. $2' \ (0,1/2,0) \ 1/4,y,1/4$
   - \[(2_y|1/2,1/2,1/2)'\]

6. $2' \ (1/2,0,0) \ x,1/4,1/4$
   - \[(2_x|1/2,1/2,1/2)'\]

7. $2' \ x,x,0$
   - \[(2_x|x,0,0)'\]

8. $2 \ x,x,0$
   - \[(2_x|x,0,0)'\]
Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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<td>16 g 1</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>(2) x,y,z</td>
</tr>
<tr>
<td>(3) y+1/2,x+1/2,z+1/2</td>
<td>(4) y+1/2,x+1/2,z+1/2</td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z+1/2</td>
<td>(6) x+1/2,y+1/2,z+1/2</td>
</tr>
<tr>
<td>(7) y,x,z</td>
<td>(8) y,x,z</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1'  
Along [1,0,0] p2a' 2mg  
Along [1,1,0] p2a' 2mm

\[ a^* = a \quad b^* = b \]
Origin at 0,1/2,z

\[ a^* = b \quad b^* = c \]
Origin at x,1/4,3/4

\[ a^* = -c \quad b^* = (-a + b)/2 \]
Origin at x,x,1/2
Origin on 2 [0,1,0] at 43 (1,2) 1

Asymmetric unit
0 ≤ x ≤ 1;
0 ≤ y ≤ 1;
0 ≤ z ≤ 1/8

Symmetry Operations

(1) 1
(1|0,0,0)

(2) 2 (0,0,1/2) 0,0,z
(2z|0,0,1/2)

(3) 4+ (0,0,3/4) 0,0,z
(4z|0,0,3/4)

(4) 4- (0,0,1/4) 0,0,z
(4z⁻¹|0,0,1/4)

(5) 2 0,y,0
(2|0,0,0)

(6) 2 x,0,1/4
(2x|0,0,1/2)

(7) 2 x,x,1/8
(2xx|0,0,1/4)

(8) 2 x,x,3/8
(2xx|0,0,3/4)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>5 x,y,z [u,v,w]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td>4 c ..2</td>
<td>x,x,5/8 [u,u,0]</td>
<td>x,x,1/8 [u,u,0]</td>
</tr>
<tr>
<td>4 b .2</td>
<td>1/2,y,0 [0,v,0]</td>
<td>1/2,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>4 a .2</td>
<td>0,y,0 [0,v,0]</td>
<td>0,y,1/2 [0,v,0]</td>
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</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] p4m'm'  
\( a^* = a \quad b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p2m'g'  
\( a^* = -c \quad b^* = b \)  
Origin at x,0,1/4

Along [1,1,0] p2m'g'  
\( a^* = -c \quad b^* = (-a + b)/2 \)  
Origin at x,x,1/8
Origin on $2 \{0,1,0\} 1'$ at $4_3 (1,2) 11'$

Asymmetric unit $\quad 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For 1 + set

(1) $1$
    (1) $0,0,0$

(2) 2 $\{0,0,1/2\}$ $0,0,z$
    (2) $z,0,0,1/2$

(3) $4^+ (0,0,3/4)$ $0,0,z$
    (4) $4^+ (0,0,1/4)$ $0,0,z$
    (4) $z,0,0,1/4$

(5) 2 $0,y,0$
    (2) $0,0,0$

(6) 2 $x,0,1/4$
    (6) $z,0,0,1/2$

(7) 2 $x,x,1/8$
    (7) $x,x,0,0,1/4$

(8) 2 $x,x,3/8$
    (8) $z,x,0,0,3/4$

For 1' + set

(1) $1'$
    (1) $0,0,0'$

(2) 2 $\{0,0,1/2\}'$ $0,0,z$
    (2) $z,0,0,1/2'$

(3) $4^+ (0,0,3/4)'$ $0,0,z$
    (4) $4^+ (0,0,1/4)'$ $0,0,z$
    (4) $z,0,0,1/4'$

(5) 2' $0,y,0$
    (2) $0,0,0'$

(6) 2 $x,0,1/4$
    (6) $z,0,0,1/2'$

(7) 2 $x,x,1/8$
    (7) $x,x,0,0,1/4'$

(8) 2 $x,x,3/8$
    (8) $z,x,0,0,3/4'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

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<th>Site Symmetry</th>
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<td>(1) x,y,z [0,0,0]</td>
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<td>x,x,3/8 [0,0,0]</td>
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<td>x,x,7/8 [0,0,0]</td>
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<tr>
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<td>y,1/2,3/4 [0,0,0]</td>
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<td>a .2.1'</td>
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<td>y,0,1/4 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4mm1'  a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2mg1'  a* = -c  b* = b
Origin at x,0,1/4

Along [1,1,0] p2mg1'  a* = -c  b* = (-a + b)/2
Origin at x,x,1/8
Origin on 2 [0,1,0] at 4 \(\frac{3}{4}\) (1,2) 1

Asymmetric unit \(0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{8}\)

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 0,0,1/2 \\
(2) & \quad (0,0,1/2) \\
(2) & \quad 0,0,0 \\
(2) & \quad (0,0,1/2) \\
(2) & \quad 0,0,0 \\
(2) & \quad (0,0,1/2) \\
(3) & \quad 4^+ \cdot (0,0,3/4) \\
(3) & \quad 0,0,z \\
(3) & \quad (4_z,0,0,3/4) \\
(3) & \quad 0,0,3/4 \\
(3) & \quad (4_z,0,0,3/4) \\
(4) & \quad 4^+ \cdot (0,0,1/4) \\
(4) & \quad 0,0,z \\
(4) & \quad (4_z,0,0,1/4) \\
(4) & \quad 0,0,1/4 \\
(5) & \quad 2^\times \cdot (0,0,0) \\
(5) & \quad 0,y,0 \\
(5) & \quad (2_z,0,0,0) \\
(5) & \quad 0,y,0 \\
(5) & \quad (2_z,0,0,0) \\
(5) & \quad (2_z,0,0,0) \\
(6) & \quad x,0,1/4 \\
(6) & \quad (2_x,0,0,1/2) \\
(6) & \quad x,0,1/4 \\
(6) & \quad (2_x,0,0,1/2) \\
(7) & \quad 2^+ \cdot x,x,1/8 \\
(7) & \quad (2_{xy},0,0,1/4) \\
(7) & \quad 2^+ \cdot x,x,1/8 \\
(7) & \quad (2_{xy},0,0,1/4) \\
(8) & \quad 2^+ \cdot x,x,3/8 \\
(8) & \quad (2_{xy},0,0,3/8) \\
(8) & \quad x,x,3/8 \\
(8) & \quad (2_{xy},0,0,3/8) \\
\end{align*}
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

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<td>4 c .2'</td>
<td>x,x,1/8 [u,u,w]</td>
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<td>x,x,3/8 [u,u,w]</td>
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<td>x,x,7/8 [u,u,w]</td>
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<td>4 b .2.</td>
<td>1/2,y,0 [0,v,0]</td>
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<td>1/2,y',1/2 [0,v',0]</td>
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Symmetry of Special Projections

Along [0,0,1] p4'm'm
\[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2'm'g'
\[ \mathbf{a}^* = -\mathbf{c}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,1/4

Along [1,1,0] p2'mg'
\[ \mathbf{a}^* = -\mathbf{c}, \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]
Origin at x,x,1/8
Origin on $2' \begin{bmatrix} 0,1,0 \end{bmatrix}$ at $4_3 \begin{bmatrix} 1,2' \end{bmatrix} 1$

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq 1/8$

Symmetry Operations

1. $1$

2. $2 \begin{bmatrix} 0,0,1/2 \end{bmatrix}$ $0,0,z$
   $2_z \begin{bmatrix} 0,0,1/2 \end{bmatrix}$

3. $4^+ \begin{bmatrix} 0,0,3/4 \end{bmatrix}$ $0,0,z$
   $4_z \begin{bmatrix} 0,0,3/4 \end{bmatrix}$

4. $4^- \begin{bmatrix} 0,0,1/4 \end{bmatrix}$ $0,0,z$
   $4_z^{-1} \begin{bmatrix} 0,0,1/4 \end{bmatrix}$

5. $2', 0,y,0$
   $2_z \begin{bmatrix} 0,0,0 \end{bmatrix}$

6. $2', x,0,1/4$
   $2_x \begin{bmatrix} 0,0,1/2 \end{bmatrix}$

7. $2', x,x,1/8$
   $2_{xy} \begin{bmatrix} 0,0,1/4 \end{bmatrix}$

8. $2', x,x,3/8$
   $2_{xy} \begin{bmatrix} 0,0,3/4 \end{bmatrix}$
Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 c .2'</td>
<td>x,x,5/8 [u,u,w]</td>
</tr>
<tr>
<td>4 b .2'</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>4 a .2'</td>
<td>0,y,0 [u,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm</th>
<th>Along [1,0,0]</th>
<th>p2'mg'</th>
<th>Along [1,1,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{a}^* = \mathbf{a} ) \quad \mathbf{b}^* = \mathbf{b}</td>
<td>( \mathbf{a}^* = -\mathbf{c} ) \quad \mathbf{b}^* = \mathbf{b}</td>
<td>( \mathbf{a}^* = -\mathbf{c} ) \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,1/4</td>
<td>Origin at x,x,1/8</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2 [0,1,0] at 4_3 (1,2) 1

Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

1. 1
2. 2 \(0,0,1/2\) 0,0,z
3. 4' \(0,0,3/4\) 0,0,z
4. 4' \(0,0,1/4\) 0,0,z
5. 2' 0,y,0
6. 2' \(x,0,1/4\)
7. 2 \(x,x,1/8\)
8. 2 \(x,x,3/8\)

P4_3 '2'2

95.5.797

P4_3 '2'2
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td>[u,v,w]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4 c ..2</td>
<td>x,x,5/8 [u,u,0]</td>
<td>x,x,1/8 [u,u,0]</td>
</tr>
<tr>
<td>4 b ..2'</td>
<td>1/2,y,0 [u,0,w]</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>4 a ..2'</td>
<td>0,y,0 [u,0,w]</td>
<td>0,y,1/2 [u,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'm'm</th>
<th>Along [1,0,0]</th>
<th>p2'mg'</th>
<th>Along [1,1,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -c</td>
<td>b* = b</td>
<td>a* = -c</td>
<td>b* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,1/4</td>
<td></td>
<td>Origin at x,x,1/8</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on 2 [0,1,0] at 4$_3$ (1,2) 1

**Asymmetric unit** \(0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8\)

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

1. \((1) 1 (1,0,0,0)\)
2. \((2) 2 (0,0,1/2) \quad 0,0,z\)
3. \((3) 4^+ (0,0,3/4) \quad 0,0,z\)
4. \((4) 4^- (0,0,1/4) \quad 0,0,z\)
5. \((5) 2 \quad 0,y,0\) \(\begin{array}{c}
(2_1,0,0,0) \\

\end{array}\)
6. \((6) 2 \quad x,0,1/4\) \(\begin{array}{c}
(2 \times 0,0,1/2) \\

\end{array}\)
7. \((7) 2 \quad x,x,1/8\) \(\begin{array}{c}
(2 \times 0,0,1/4) \\

\end{array}\)
8. \((8) 2 \quad x,x,3/8\) \(\begin{array}{c}
(2 \times 0,0,3/4) \\

\end{array}\)

For \((1,0,0)^' + \text{ set}\)

1. \((1) t' (1,0,0)^'\) \(\begin{array}{c}
(1,1,0,0)^' \\

\end{array}\)
2. \((2) 2 (0,0,1/2) \quad 1/2,0,z\) \(\begin{array}{c}
(2 \times 1,0,1/2)^' \\

\end{array}\)
3. \((3) 4^+ (0,0,3/4) \quad 1/2,1/2,z\) \(\begin{array}{c}
(4 \times 1,0,3/4)^' \\

\end{array}\)
4. \((4) 4^- (0,0,1/4) \quad 1/2,-1/2,z\) \(\begin{array}{c}
(4 \times 1,0,1/4)^' \\

\end{array}\)
5. \((5) 2^' \quad 1/2,y,0\) \(\begin{array}{c}
(2_1,1,0,0)^' \\

\end{array}\)
6. \((6) 2^' (1,0,0) \quad x,0,1/4\) \(\begin{array}{c}
(2 \times 1,0,1/2)^' \\

\end{array}\)
7. \((7) 2^' (1/2,1/2,0) \quad x+1/2,x,1/8\) \(\begin{array}{c}
(2 \times 1,0,1/4)^' \\

\end{array}\)
8. \((8) 2^' (1/2,-1/2,0) \quad x+1/2,x,3/8\) \(\begin{array}{c}
(2 \times 1,0,3/4)^' \\

\end{array}\)
**Generators selected**

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>16 1</td>
<td></td>
</tr>
<tr>
<td>16 1 d</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 1 d</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>16 1 d</td>
<td>(3) y,x,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td>16 1 d</td>
<td>(4) y,x,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>16 1 x</td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 1 x</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>16 1 x</td>
<td>(7) y,x,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>16 1 x</td>
<td>(8) y,x,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td>8 c</td>
<td>x,x,5/8 [u,u,0]</td>
</tr>
<tr>
<td>8 c .2</td>
<td>x,x,1/8 [u,u,0]</td>
</tr>
<tr>
<td>8 c .2</td>
<td>x,x,3/8 [u,u,0]</td>
</tr>
<tr>
<td>8 c .2</td>
<td>x,x,7/8 [u,u,0]</td>
</tr>
<tr>
<td>8 b .2'</td>
<td>1/2,y,0 [u,0,w]</td>
</tr>
<tr>
<td>8 b .2'</td>
<td>1/2,y,1/2 [u,0,w]</td>
</tr>
<tr>
<td>8 b .2'</td>
<td>y,1/2,3/4 [0,u,w]</td>
</tr>
<tr>
<td>8 b .2'</td>
<td>y,1/2,1/4 [0,u,w]</td>
</tr>
<tr>
<td>8 a .2</td>
<td>0,y,0 [0,v,0]</td>
</tr>
<tr>
<td>8 a .2</td>
<td>0,y,1/2 [0,v,0]</td>
</tr>
<tr>
<td>8 a .2</td>
<td>y,0,3/4 [v,0,0]</td>
</tr>
<tr>
<td>8 a .2</td>
<td>y,0,1/4 [v,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p<sub>c</sub> 4mm' a<sup>*</sup> = a b<sup>*</sup> = b

Along [1,0,0] p2mg1' a<sup>*</sup> = -c b<sup>*</sup> = b

Along [1,1,0] p<sub>2v</sub> 2m'g' a<sup>*</sup> = -c b<sup>*</sup> = (-a + b)/2

Origin at 0,0,z

Origin at x,0,1/4

Origin at x,x,1/8
Origin on \([0,1,0]\) at \(4_3\) \((1,2) 1\)

Asymmetric unit \(0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8\)

Symmetry Operations

For \((0,0,0) + \) set

(1) \(1 \quad (1|0,0,0)\)
(2) \(2 (0,0,1/2) \quad 0,0,z \quad (2_z|0,0,1/2)\)
(3) \(4^+ \cdot (0,0,3/4) \quad 0,0,z \quad (4_z|0,0,3/4)\)
(4) \(4^- \cdot (0,0,1/4) \quad 0,0,z \quad (4_z^-|0,0,1/4)\)

For \((1,0,0) + \) set

(1) \(t' (1,0,0) \quad (1|1,0,0)\)
(2) \(2' (0,0,1/2) \quad 1/2,0,z \quad (2_z|1,0,1/2)\)
(3) \(4^+ (0,0,3/4) \quad 1/2,1/2,z \quad (4_z|1,0,3/4)\)
(4) \(4^- (0,0,1/4) \quad 1/2,-1/2,z \quad (4_z^-|1,0,1/4)\)

(5) \(2' 1/2,y,0 \quad (2_z|1,0,0)\)
(6) \(2' (1,0,0) \quad x,0,1/4 \quad (2_x|1,0,1/2)\)
(7) \(2 x+1/2,x,1/8 \quad (2_{xy}|1,0,1/4)\)
(8) \(2 x+1/2,x,3/8 \quad (2_{xy}|1,0,3/4)\)
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
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<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>16 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(3) y, x, z + 3/4 [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(4) y, x, z + 1/4 [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(6) x, y, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(7) y, x, z + 1/4 [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(8) y, x, z + 3/4 [v, u, w]</td>
</tr>
<tr>
<td>8 c ..2'</td>
<td>x, x, 5/8 [u, u, w]</td>
</tr>
<tr>
<td></td>
<td>x, x, 1/8 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>x, x, 3/8 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>x, 7/8 [u, u, w]</td>
</tr>
<tr>
<td>8 b .2'</td>
<td>1/2, y, 0 [u, 0, w]</td>
</tr>
<tr>
<td></td>
<td>1/2, y, 1/2 [u, 0, w]</td>
</tr>
<tr>
<td></td>
<td>y, 1/2, 3/4 [0, u, w]</td>
</tr>
<tr>
<td></td>
<td>y, 1/2, 1/4 [0, u, w]</td>
</tr>
<tr>
<td>8 a .2.</td>
<td>0, y, 0 [0, v, 0]</td>
</tr>
<tr>
<td></td>
<td>0, y, 1/2 [0, v, 0]</td>
</tr>
<tr>
<td></td>
<td>y, 0, 3/4 [v, 0, 0]</td>
</tr>
<tr>
<td></td>
<td>y, 0, 1/4 [v, 0, 0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] pₜₜ 4m'm'

a* = a   b* = b
Origin at 0,0,z

Along [1,0,0] p2mg1'

a* = -c   b* = b
Origin at x,0,1/4

Along [1,1,0] p₂ᵥ₂ 2mg

a* = -c   b* = (-a + b)/2
Origin at x,x,1/8
Origin on 2 [1,1,0] at 2, 1 (1,2)

Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

1. 1 (0,0,0)
   (1) 0,0,0

2. 2 (0,0,1/2) 0,0,z
   (2) 0,0,1/2
   (3) 4+ (0,0,3/4) 0,1/2,z
   (4) 4- (0,0,1/4) 1/2,0,z
   (4-z) 1/2,1/2,3/4
   (4-z) 1/2,1/2,1/4

3. 2 (1/2,0,0) x,1/4,1/8
   (5) 1/2,1/2,1/2,1/4
   (6) 1/2,1/2,3/4

4. 2 x,x,0
   (x) 0,0,0
   (7) x,x,0
   (2x) 0,0,1/2

5. 2 (0,1/2,0) 1/4,y,3/8
   (2y) 1/2,1/2,1/4

6. 2 (1/2,1/2,1/2) 0,0,0
   (xy) 0,0,1/2

Tetragonal

P4₁₂₂
96.1.800
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+3/4 [v,w]</td>
<td>(4) y+1/2,x+1/2,z+1/4 [v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+3/4 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/4 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 a .2</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x+1/2,3/4 [u,u,0]</td>
<td>x+1/2,x+1/2,1/4 [u,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4g'm'  
\(\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,1/2,z

Along [1,0,0] p2'gg'  
\(\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at x,1/4,1/8

Along [1,1,0] p2m'g'  
\(\mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)  
Origin at x,x,0
Origin on 2 $[1,1,0]1'$ at 2, 1 $(1,2)1'$

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $1 +$ set

1. $1$
   1. $0,0,0$

5. $2 (0,1/2,0) \quad 1/4,y,3/8$
   2. $(2_y,1/2,1/2,3/4)$

For $1' +$ set

1. $1'$
   1. $0,0,0'$

5. $2' (0,1/2,0) \quad 1/4,y,3/8$
   2. $(2_y,1/2,1/2,3/4)'$
**Generators selected**

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2): (3); (5); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>b</th>
<th>11'</th>
<th>(1) x,y,z [0,0,0]</th>
<th>(2) x,y,z+1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) y+1/2,x+1/2,z+3/4 [0,0,0]</td>
<td>(4) x+1/2,y+1/2,z+1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) x+1/2,y+1/2,z+3/4 [0,0,0]</td>
<td>(6) y+1/2,x+1/2,z+1/4 [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(7) y,x, 0 [0,0,0]</td>
<td>(8) y,x, z+1/2 [0,0,0]</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>a</th>
<th>.21'</th>
<th>(1) x,x,0 [0,0,0]</th>
<th>(2) x,x,1/2 [0,0,0]</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>x+1/2,x+1/2,3/4 [0,0,0]</td>
<td>x+1/2,x+1/2,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p4gm1'
  - $a^* = a$  $b^* = b$
- Along [1,0,0] p2gg1'
  - $a^* = b$  $b^* = c$
- Along [1,1,0] p2mg1'
  - $a^* = -c$  $b^* = (-a + b)/2$

Origin at $0,1/2,z$
 Origin at $x,1/4,1/8$
 Origin at $x,x,0$
Origin on 2' [1,1,0] at 2, 1 (1,2')

Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

(1) 1
(1') 0,0,0

(2) 2 (0,0,1/2) 0,0,z
(2') 0,0,1/2

(3) 4' (0,0,3/4) 0,1/2,z
(4' y) 1/2,1/2,1/4

(4) 4' (0,0,1/4) 1/2,0,z
(4' z) 1/2,1/2,1/4

(5) 2 (0,1/2,0) 1/4,y,3/8
(5') 1/2,1/2,3/4

(6) 2 (1/2,0,0) x,1/4,1/8
(6') 1/2,1/2,1/4

(7) 2' x,x,0
(7') 0,0,0'

(8) 2' x,x,1/4
(8') 0,0,1/2'
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tr>
<td><strong>8 b 1</strong></td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td></td>
<td>(3) y+1/2,x+1/2,z+3/4 [v,u,w]</td>
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<td>(4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z+3/4 [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z+1/4 [u,v,w]</td>
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<td>(7) y,x,z+3/4 [v,u,w]</td>
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<td>(8) y,x,z+1/2 [v,u,w]</td>
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<tr>
<td><strong>4 a .2'</strong></td>
<td>x,x,0 [u,u,w]</td>
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<tr>
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<td>x,x,1/2 [u,u,w]</td>
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<tr>
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<tr>
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<td>x+1/2,x+1/2,1/4 [u,u,w]</td>
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</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**    p4'gm'  
  \( a^* = a \quad b^* = b \)

- **Along [1,0,0]**    p2g'g'  
  \( a^* = b \quad b^* = c \)

- **Along [1,1,0]**    p2m'g'  
  \( a^* = -c \quad b^* = (-a + b)/2 \)

Origin at 0,1/2,z  
Origin at x,1/4,1/8  
Origin at x,x,0
**Origin** on 2' [1,1,0] at 2, 1 (1,2')

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8 \]

**Symmetry Operations**

1. \( 1 \)
   \[ \begin{array}{c} (1) \ 1 \\ (1) \ 0,0,0 \end{array} \]

2. \( 2 \)
   \[ \begin{array}{c} (2) \ 2 \ (0,0,1/2) \ 0,0,z \\ (2) \ 0,0,1/2 \end{array} \]

3. \( 4' \)
   \[ \begin{array}{c} (3) \ 4' \ (0,0,3/4) \ 0,1/2,z \\ (4z) \ |1/2,1/2,3/4| \end{array} \]

4. \( 4 \)
   \[ \begin{array}{c} (4) \ 4' \ (0,0,1/4) \ 1/2,0,z \\ (4z^{-1}) \ |1/2,1/2,1/4| \end{array} \]

5. \( 2' \)
   \[ \begin{array}{c} (5) \ 2' \ (0,1/2,0) \ 1/4,y,3/8 \\ (2y) \ |1/2,1/2,3/4|' \end{array} \]

6. \( 2' \)
   \[ \begin{array}{c} (6) \ 2' \ (1/2,0,0) \ x,1/4,1/8 \\ (2x) \ |1/2,1/2,1/4|' \end{array} \]

7. \( 2' \)
   \[ \begin{array}{c} (7) \ 2' \ x,x,0 \\ (2xy) \ |0,0,0|' \end{array} \]

8. \( 2' \)
   \[ \begin{array}{c} (8) \ 2' \ x,x,1/4 \\ (2xy) \ |0,0,1/2|' \end{array} \]
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<td>x,y,z [u,v,w]</td>
<td>(2) x,y,z+1/2 [u,v,w]</td>
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<td>(3) y+1/2,x+1/2,z+3/4 [u,v,w]</td>
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<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
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</table>

### Symmetry of Special Projections

Along [0,0,1] p4g'm'

- a^* = a
- b^* = b

Origin at 0,1/2,z

Along [1,0,0] p2g'g'

- a^* = b
- b^* = c

Origin at x,1/4,1/8

Along [1,1,0] p2'mg'

- a^* = -c
- b^* = (-a + b)/2

Origin at x,x,0
Origin on 2 [1,1,0] at 2, 1 (1,2)

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

1. $1$
2. $2 (0,0,1/2) \quad 0,0,z$
3. $4' (0,0,3/4) \quad 0,1/2,z$
4. $4' (0,0,1/4) \quad 1/2,0,z$
5. $2' (0,1/2,0) \quad 1/4,y,3/8$
6. $2' (1/2,0,0) \quad x,1/4,1/8$
7. $x,x,0$
8. $x,x,1/4$

$\sigma$-operation:

1. $(1|0,0,0)$
2. $(2_1|0,0,1/2)$
3. $(4_z|1/2,1/2,3/4)^*$
4. $(4_z^{-1}|1/2,1/2,1/4)^*$
5. $(2_2|1/2,1/2,3/4)^*$
6. $(2_1|1/2,1/2,1/4)^*$
7. $(2_{xy}|0,0,0)$
8. $(2_{xy}|0,0,1/2)$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>4 a ..2</td>
<td>$x,x,0 [u,u,0]$</td>
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Symmetry of Special Projections

Along [0,0,1]  p4'g'm  
\( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,1/2,z

Along [1,0,0]  p2'gg'  
\( \mathbf{a}^* = -\mathbf{c} \)  \( \mathbf{b}^* = \mathbf{b} \)  
Origin at x,1/4,1/8

Along [1,1,0]  p2m'g'  
\( \mathbf{a}^* = -\mathbf{c} \)  \( \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)  
Origin at x,x,0
Origin on 422

Asymmetric unit
\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{4} \]

Symmetry Operations

For \((0,0,0) + \) set

1. \((1)\) \(1\)
   \((1,0,0,0)\)

2. \((2)\) 0,0,z
   \((2_z,0,0,0)\)

3. \((4)\) 0,0,z
   \((4_z,0,0,0)\)

4. \((4)\) 0,0,z
   \((4_z^{-1},0,0,0)\)

5. \((5)\) 0,y,0
   \((2_y,0,0,0)\)

6. \((6)\) x,0,0
   \((2_x,0,0,0)\)

7. \((7)\) x,x,0
   \((2_{xx},0,0,0)\)

8. \((8)\) x,x,0
   \((2_{xx},0,0,0)\)

For \((1/2,1/2,1/2) + \) set

1. \((1)\) t (1/2,1/2,1/2)
   \((1,1/2,1/2,1/2)\)

2. \((2)\) 0,0,1/2
   \((2_z,1/2,1/2,1/2)\)

3. \((3)\) 0,0,1/2
   \((4_z,1/2,1/2,1/2)\)

4. \((4)\) 0,0,1/2
   \((4_z^{-1},1/2,1/2,1/2)\)

5. \((5)\) (0,1/2,0)
   \((2_y,1/2,1/2,1/2)\)

6. \((6)\) 1/4,1/4,0
   \((2_x,1/2,1/2,1/2)\)

7. \((7)\) 1/4,1/4,0
   \((2_{xy},1/2,1/2,1/2)\)

8. \((8)\) 1/4,1/4,0
   \((2_{xy},1/2,1/2,1/2)\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tr>
<th>Positions</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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<td>(1/2,1/2,1/2) +</td>
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<td>x,x+1/2,1/4 [u,u,0]</td>
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<td>x,0,0 [u,0,0]</td>
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<td>0,x,0 [0,u,0]</td>
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<td>8 g .2</td>
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<td>x,x,0 [u,u,0]</td>
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<td>x,x,0 [u,u,0]</td>
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<td>1/2,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4m'm'
Along [1,0,0] c2m'm'
Along [1,1,0] p2m'm'
a* = (a - b)/2 b* = (a + b)/2
a* = b b* = c
a* = - (a + b)/2 b* = c/2
Origin at 0,0,z
Origin at x,0,0
Origin at x,x,0
Origin on 4221'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\)

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad \begin{pmatrix} 0 \ 0 \ 0 \end{pmatrix} \\
(3) & \quad \begin{pmatrix} 0 \ 0 \ z \end{pmatrix} \\
(4) & \quad \begin{pmatrix} 0 \ 0 \ -z \end{pmatrix} \\
(5) & \quad \begin{pmatrix} 0 \ y \ 0 \end{pmatrix} \\
(6) & \quad \begin{pmatrix} x \ 0 \ 0 \end{pmatrix} \\
(7) & \quad \begin{pmatrix} x \ x \ 0 \end{pmatrix} \\
(8) & \quad \begin{pmatrix} x \ y \ 0 \end{pmatrix}
\end{align*}
\]

For \((1/2,1/2,1/2)\) + set

\[
\begin{align*}
(1) & \quad t \begin{pmatrix} 1/2 \ 1/2 \ 1/2 \end{pmatrix} \\
(2) & \quad \begin{pmatrix} 0 \ 0 \ 1/2 \end{pmatrix} \\
(3) & \quad \begin{pmatrix} 0 \ 0 \ 1/2 \end{pmatrix} \\
(4) & \quad \begin{pmatrix} 0 \ 0 \ 1/2 \end{pmatrix} \\
(5) & \quad \begin{pmatrix} 0 \ y \ 0 \end{pmatrix} \\
(6) & \quad \begin{pmatrix} 1/4 \ 1/4 \ 0 \end{pmatrix} \\
(7) & \quad \begin{pmatrix} 1/4 \ 1/4 \ 0 \end{pmatrix} \\
(8) & \quad \begin{pmatrix} x \ x \ 1/4 \end{pmatrix}
\end{align*}
\]
Continued

For (0,0,0)' + set

(1) \(1'\) \((0,0,0)\) \(1'\)  
(2) \(2'\) 0,0,0  
(3) \(4'\) 0,0,0  
(4) \(4'\) 0,0,0  

(5) \(2'\) 0,y,0  
(6) \(2'\) x,0,0  
(7) \(2'\) x,x,0  
(8) \(2'\) x,x,0  

For (1/2,1/2,1/2)' + set

(1) \(t(1/2,1/2,1/2)\) \(t(1/2,1/2,1/2)\)  
(2) \(2'(1/2,0,0)\) x,1/4,1/4  
(3) \(2'(1/2,1/2,0)\) x,x,1/4  
(4) \(2'(1/2,1/2,1/2)\) x,x,1/4  

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

Multiplicity  Coordinates

<table>
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<tr>
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<th>Coordinates</th>
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<td>(1) x,y,z [0,0,0]</td>
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<td>(4) x,y,z [0,0,0]</td>
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<td>(12) x,0,1/2 [0,0,0]</td>
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<td>(39) 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(40) 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 4221'</td>
<td>(41) 0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(42) 0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(43) 0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(44) 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>c2mm1'</th>
<th>Along [1,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -(a + b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on 4'22'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 4^+ \quad 0,0,z \\
(4) & \quad 4^- \quad 0,0,z
\end{align*}
\]

\[
\begin{align*}
(1) & \quad (1,0,0,0) \\
(2) & \quad (2,0,0) \\
(3) & \quad (4_z,0,0,0) \\
(4) & \quad (4_z^{-1},0,0,0)
\end{align*}
\]

\[
\begin{align*}
(5) & \quad 2 \quad 0,y,0 \\
(6) & \quad 2 \quad x,0,0 \\
(7) & \quad 2' \quad x,x,0 \\
(8) & \quad 2' \quad x,0,0,0
\end{align*}
\]

\[
\begin{align*}
(5) & \quad (2,0,0,0) \\
(6) & \quad (2,0,0,0) \\
(7) & \quad (2,0,0,0) \\
(8) & \quad (2,0,0,0)
\end{align*}
\]

For \((1/2,1/2,1/2) + \) set

\[
\begin{align*}
(1) & \quad t \quad (1/2,1/2,1/2) \\
(2) & \quad 2 \quad (0,0,1/2) \quad 1/4,1/4,z \\
(3) & \quad 4^+ \quad (0,0,1/2) \quad 0,1/2,z \\
(4) & \quad 4^- \quad (0,0,1/2) \quad 1/2,0,z
\end{align*}
\]

\[
\begin{align*}
(5) & \quad (1/2,1/2,1/2) \\
(6) & \quad (1/2,0,0) \quad x,1/4,1/4 \\
(7) & \quad 2' \quad (1/2,1/2,0) \quad x,x,1/4 \\
(8) & \quad 2' \quad x,x + 1/2,1/4
\end{align*}
\]

\[
\begin{align*}
(5) & \quad (1/2,1/2,1/2) \\
(6) & \quad (1/2,1/2,1/2) \\
(7) & \quad (1/2,1/2,1/2) \\
(8) & \quad (1/2,1/2,1/2)
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>k</td>
<td>1</td>
</tr>
</tbody>
</table>

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

(1) x,y,z [u,v,w] (2) x,y,z [v,u,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w]

8 j .2' x,x+1/2,1/4 [u,u,w] x+1/2,x,1/4 [u,u,w] x+1/2,x,1/4 [u,u,w]

8 i .2' x,0,1/2 [u,0,0] 0,x,1/2 [0,u,0] 0,x,1/2 [0,u,0]

8 h .2' x,0,0 [u,0,0] 0,x,0 [0,u,0] 0,x,0 [0,u,0]

8 g .2' x,x,0 [u,u,w] x,x,0 [u,u,w] x,x,0 [u,u,w]

8 f .2' 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z [0,0,w]

4 e .4' 0,0,z [0,0,0] 0,0,z [0,0,0]

4 d 2.2' 0,1/2,1/4 [0,0,w] 1/2,0,1/4 [0,0,w]

4 c 222. 0,1/2,0 [0,0,0] 1/2,0,0 [0,0,0]

2 b 4'22' 0,0,1/2 [0,0,0]

2 a 4'22' 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4m'm' Along [1,0,0] c2m'm' Along [1,1,0] p2mm'

\( a^* = (a - b)/2 \quad b^* = (a + b)/2 \)

Origin at 0,0,z

\( a^* = b \quad b^* = c \)

Origin at x,0,0

\( a^* = -c/2 \quad b^* = (-a + b)/2 \)

Origin at x,x,0
Origin on 42'2'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)
(2) 2 0,0,z (2z|0,0,0)
(3) 4' 0,0,z (4z|0,0,0)
(4) 4' 0,0,z (4z'|0,0,0)
(5) 2' 0,y,0 (2y|0,0,0)
(6) 2' x,0,0 (2x|0,0,0)
(7) 2' x,x,0 (2x|0,0,0)
(8) 2' x,x,0 (2x|0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (1|1/2,1/2,1/2)
(2) 2 (0,0,1/2) 1/4,1/4,z (2z|1/2,1/2,1/2)
(3) 4' (0,0,1/2) 0,1/2,z (4z|1/2,1/2,1/2)
(4) 4' (0,0,1/2) 1/2,0,z (4z'|1/2,1/2,1/2)
(5) 2' (0,1/2,0) 1/4,y,1/4 (2y|1/2,1/2,1/2)
(6) 2' (1/2,0,0) x,1/4,1/4 (2x|1/2,1/2,1/2)
(7) 2' (1/2,1/2,0) x,x,1/4 (2x|1/2,1/2,1/2)
(8) 2' x,x+1/2,1/4 (2x|1/2,1/2,1/2)
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16  k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8  j .2'</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
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<tr>
<td></td>
<td>x,x+1/2,1/4 [u,u,w]</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td>8  i .2'</td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>8  h .2'</td>
<td>x,0,0 [0,v,w]</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [0,v,w]</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>8  g .2'</td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td>8  f 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4  e 4..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4  d 2.2'</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4  c 22'2'</td>
<td>0,1/2,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2  b 42'2'</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2  a 42'2'</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm

Along [1,0,0] c2'mm'

Along [1,1,0] p2'mm'

\[
a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2}
\]

Origin at 0,0,z

\[
a^* = -c/b \quad b^* = b
\]

Origin at x,0,0

\[
a^* = -c/2 \quad b^* = (-a + b)/2
\]

Origin at x,x,0
Origin on 4'2'2

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1(0,0,0)\)
2. \(r,0,0\)
3. \(4,0,0\)
4. \(4,0,0\)
5. \(2,0,0\)
6. \(2,0,0\)
7. \(2,0,0\)
8. \(2,0,0\)

For \((1/2,1/2,1/2) + \) set

1. \(1(1/2,1/2,1/2)\)
2. \(2(1/2,1/2,1/2)\)
3. \(4,0,0\)
4. \(4,0,0\)
5. \(2,0,0\)
6. \(2,0,0\)
7. \(2,0,0\)
8. \(2,0,0\)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>k</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>j</td>
<td>x,x+1/2,1/4 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>i</td>
<td>x,0,1/2 [0,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>h</td>
<td>x,0,0 [0,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>g</td>
<td>x,0,0 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>0,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>0,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>0,1/2,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm' 
\[ a^* = (a - b)/2 \quad \text{and} \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] c2mm' 
\[ a^* = -c \quad \text{and} \quad b^* = b \]
Origin at x,0,0

Along [1,1,0] p2m'm' 
\[ a^* = -(a + b)/2 \quad \text{and} \quad b^* = c/2 \]
Origin at x,x,0
Origin on 422

Asymmetric unit \( 0 \leq x \leq \frac{1}{2}; \ 0 \leq y \leq \frac{1}{2}; \ 0 \leq z \leq \frac{1}{4} \)

Symmetry Operations

For \((0,0,0) + \) set

1. \((1) \ 1 (0,0,0)\)
2. \((2) \ 0,0,z \)
   \( (2z) (0,0,0) \)
3. \((3) \ 4^+ 0,0,z \)
   \( (4z) (0,0,0) \)
4. \((4) \ 4^- 0,0,z \)
   \( (4z^-1) (0,0,0) \)

For \((1/2,1/2,1/2)' + \) set

1. \((1) \ t' (1/2,1/2,1/2) \)
   \( (1/2,1/2,1/2)' \)
2. \((2) \ 2' (0,0,1/2) \)
   \( 1/4,1/4,z \)
   \( (2z) (1/2,1/2,1/2)' \)
3. \((3) \ 4'^+ (0,0,1/2) \)
   \( 0,1/2,z \)
   \( (4z) (1/2,1/2,1/2)' \)
4. \((4) \ 4'^- (0,0,1/2) \)
   \( 1/2,0,z \)
   \( (4z^-1) (1/2,1/2,1/2)' \)

For \((1/2,1/2,1/2)' + \) set

1. \((1) \ t' (1/2,1/2,1/2) \)
   \( (1/2,1/2,1/2)' \)
2. \((2) \ 2' (1/2,0,0) \)
   \( x,1/4,1/4 \)
   \( (2z) (1/2,1/2,1/2)' \)
3. \((3) \ 4'^+ (1/2,1/2,2,0) \)
   \( x,x,1/4 \)
   \( (2z) (1/2,1/2,1/2)' \)
4. \((4) \ 4'^- (1/2,1/2,2,0) \)
   \( x,\bar{x}+1/2,1/4 \)
   \( (2z) (1/2,1/2,1/2)' \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2)′ +</td>
</tr>
<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 j .2'</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td>8 i .2.</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 h .2.</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>8 g .2</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>8 f .2.</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 4..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 d 2.2′2′</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4 c 222.</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b 422</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 422</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_p 4m'm' \) \( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)
Origin at 0,0,z

Along [1,0,0] \( c_p 2m'm' \) \( a^* = b \) \( b^* = c \)
Origin at x,0,0

Along [1,1,0] \( p_{2c} 2m'm' \) \( a^* = -c/2 \) \( b^* = (-a + b)/2 \)
Origin at x,x,0
Origin on 4'22'

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

For \((0,0,0) + \) set

(1) 1
(1 \(0,0,0\))

(2) \(2 \quad 0,0,z\)
(2\(z\) \(0,0,0\))

(3) \(4^+ \quad 0,0,z\)
(4\(z\) \(0,0,0\)')

(4) \(4^- \quad 0,0,z\)
(4\(z\) \(-1\) \(0,0,0\)')

(5) \(2' \quad 0,y,0\)
(2\(y\) \(0,0,0\))

(6) \(2' \quad x,0,0\)
(2\(x\) \(0,0,0\))

(7) \(2' \quad x,x,0\)
(2\(xy\) \(0,0,0\)')

(8) \(2' \quad x,x,0\)
(2\(xy\) \(0,0,0\)')

For \((1/2,1/2,1/2)' + \) set

(1) \(t' \quad (1/2,1/2,1/2)\)
(1 \(1/2,1/2,1/2\)')

(2) \(2' \quad (0,0,1/2)\)
(2\(z\) \(1/2,1/2,1/2\)')

(3) \(4^+ \quad (0,0,1/2)\)
(4\(z\) \(1/2,1/2,1/2\)')

(4) \(4^- \quad (0,0,1/2)\)
(4\(z\) \(-1\) \(1/2,1/2,1/2\)')

(5) \(2' \quad (0,1/2,0)\)
(2\(y\) \(1/2,1/2,1/2\))

(6) \(2' \quad (1/2,0,0)\)
(2\(x\) \(1/2,1/2,1/2\)')

(7) \(2 \quad (1/2,1/2,0)\)
(2\(xy\) \(1/2,1/2,1/2\)')

(8) \(2 \quad x,x+1/2,1/4\)
(2\(xy\) \(1/2,1/2,1/2\)')

97.7.811 - 1 - 1615
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'((1/2,1/2,1/2)); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Generators</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
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<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td>(1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
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<tr>
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<td>(4) y,x,z [v,u,w]</td>
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</tr>
<tr>
<td>8 j</td>
<td>2</td>
<td>x,x+1/2,1/4 [u,u,0]</td>
<td>x+1/2,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td>8 i</td>
<td>2</td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td>8 h</td>
<td>2</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
<td>8 g</td>
<td>2</td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td>8 f</td>
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<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e</td>
<td>4'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 d</td>
<td>22.2</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c</td>
<td>222.</td>
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<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b</td>
<td>4'22'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a</td>
<td>4'22'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p\textsubscript{\textgamma} 4m\textgamma m'

\( \mathbf{a}^* = \frac{(a - b)}{2} \quad \mathbf{b}^* = \frac{(a + b)}{2} \)

Origin at 0,1/2,z

Along [1,0,0] c\textsubscript{\textgamma} 2m\textgamma m'

\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)

Origin at x,0,0

Along [1,1,0] p\textsubscript{2\textgamma} 2m\textgamma m'

\( \mathbf{a}^* = -\frac{c}{2} \quad \mathbf{b}^* = \frac{-(a + b)}{2} \)

Origin at x,x,1/4
**Origin** on 42’2’

**Asymmetric unit** 
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

**Symmetry Operations**

For (0,0,0) + set

(1) 1  
(2) 2' 0,0,z  
(3) 4+ 0,0,0  
(4) 4' 0,0,z  

(5) 2' 0,y,0  
(6) 2' x,0,0  
(7) 2' x,x,0  
(8) 2' x,x,0  

For (1/2,1/2,1/2)’ + set

(1) t' (1/2,1/2,1/2)’  
(2) 2' (0,0,1/2) 1/4,1/4,z  
(3) 4+’ (0,0,1/2) 0,1/2,z  
(4) 4’ (0,0,1/2) 1/2,0,z  

(5) 2 (0,1/2,0) 1/4,y,1/4  
(6) 2 (1/2,0,0) x,1/4,1/4  
(7) 2 (1/2,1/2,0) x,x,1/4  
(8) 2 x,x+1/2,1/4  

97.8.812 - 1 - 1617
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,1/2)'</td>
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#### Positions Table

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<tr>
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<td>(4) y,x,z [v,u,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
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<tr>
<td>8 j</td>
<td>.2</td>
<td>x,x+1/2,1/4 [u,u,0]</td>
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<tr>
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<td>.2'</td>
<td>x,0,1/2 [0,v,w]</td>
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<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>.2'</td>
<td>x,0,0 [0,v,w]</td>
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<td></td>
<td>x,0,0 [0,v,w]</td>
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<tr>
<td>8 g</td>
<td>.2'</td>
<td>x,x,0 [u,u,w]</td>
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<td>x,x,0 [u,u,w]</td>
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<tr>
<td>8 f</td>
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<td>0,1/2,z [0,0,w]</td>
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<td>0,1/2,z [0,0,w]</td>
</tr>
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<td>4 e</td>
<td>4'</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 d</td>
<td>2,2'</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
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<td></td>
<td>1/2,0,1/4 [0,0,0]</td>
</tr>
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<td>1/2,0,0 [0,0,w]</td>
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<tr>
<td>2 b</td>
<td>42'</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a</td>
<td>42'</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

#### Symmetry of Special Projections

- **Along [0,0,1]** $p_{\text{p'}}4\text{mm}$
  - $a^* = (a - b)/2$
  - $b^* = (a + b)/2$
- **Along [1,0,0]** $c_{\text{p'}}2\text{mm'}$
  - $a^* = -c$
  - $b^* = b$
- **Along [1,1,0]** $p_{2\text{c}}2\text{m'm'}$
  - $a^* = -c/2$
  - $b^* = (-a + b)/2$

Origin at 0,0,z

Origin at x,0,0

Origin at x,x,1/4
**Origin** on 4'2'2

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \((1) 1 \quad (1 | 0,0,0)\)
2. \((2) \quad 0,0,z \quad (2 | 0,0,0)\)
3. \((3) \quad 4^* \quad 0,0,z \quad (4 | 0,0,0)'\)
4. \((4) \quad 4^- \quad 0,0,z \quad (4 | 0,0,0)'\)

For \((1/2,1/2,1/2)' + \text{set}\)

1. \((1) 1' \quad (1/2,1/2,1/2)'\)
2. \((2) \quad 0,0,1/2 \quad 1/4,1/4,z \quad (2 | 1/2,1/2,1/2)'\)
3. \((3) \quad 4^* \quad 0,0,1/2 \quad 0,1/2,z \quad (4 | 1/2,1/2,1/2)'\)
4. \((4) \quad 4^- \quad 0,0,1/2 \quad 1/2,0,z \quad (4 | 1/2,1/2,1/2)'\)

For \((1/2,1/2,1/2)' + \text{set}\)

1. \((5) 2' \quad 0,y,0 \quad (2 | 0,0,0)'\)
2. \((6) \quad x,0,0 \quad (2 | 0,0,0)'\)
3. \((7) \quad 2' \quad x,x,0 \quad (2 | 0,0,0)'\)
4. \((8) \quad 2' \quad x,x,0 \quad (2 | 0,0,0)'\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
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<tr>
<td>8 j .2'</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td>8 i .2'</td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
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<tr>
<td>8 h .2'</td>
<td>x,0,0 [u,u,0]</td>
<td>x,0,0 [u,u,0]</td>
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<tr>
<td>8 g .2</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
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<tr>
<td>8 f 2..</td>
<td>0,1/2, z [0,0,w]</td>
<td>1/2,0, z [0,0,w]</td>
</tr>
<tr>
<td>4 e 4'..</td>
<td>0,0, z [0,0,0]</td>
<td>0,0, z [0,0,0]</td>
</tr>
<tr>
<td>4 d 2.2'</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>1/2,0,1/4 [0,0,w]</td>
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<td>4 c 22'</td>
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<td>1/2,0,0 [0,0,w]</td>
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<tr>
<td>2 b 4'2'</td>
<td>0,0, 1/2 [0,0,0]</td>
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<tr>
<td>2 a 4'2'</td>
<td>0,0, 0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_4' 4m'm'  
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,1/2, z

Along [1,0,0] c_p 2mm'  
\[ a^* = -c \quad b^* = b \]
Origin at x,0,0

Along [1,1,0] p_2c 2m'm'  
\[ a^* = -c/2 \quad b^* = -(a + b)/2 \]
Origin at x,x,0
Origin at 222 at 212

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\)
2. \((0,0,0)\)
3. \((0,0,1/4)\)
4. \((0,0,1/4)\)

For \((1/2,1/2,1/2) + \) set

1. \(t\)
2. \((1/2,0,1/2)\)
3. \((1/2,0,1/2)\)
4. \((1/2,0,1/2)\)

For \((1/2,1/2,1/2) + \) set

1. \(t\)
2. \((1/2,0,1/2)\)
3. \((1/2,0,1/2)\)
4. \((1/2,0,1/2)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tbody>
<tr>
<td>16 g</td>
<td>(1) x,y,z  [u,v,w] (2) x, y, z  [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y, x+1/2, z+1/4  [v,u,w] (4) y, x+1/2, z+1/4  [v,u,w]</td>
</tr>
<tr>
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<td>(5) x, y+1/2, z+1/4  [u,v,w] (6) x, y+1/2, z+1/4  [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y, x, z  [v,u,w] (8) y, x, z  [v,u,w]</td>
</tr>
</tbody>
</table>

8 f .2. x,1/4,1/8  [u,0,0]  x,3/4,1/8  [u,0,0]  1/4,x,7/8  [0,u,0]  3/4,x,7/8  [0,u,0] |

8 e ..2 x,x,0  [u,u,0]  x,x,0  [u,u,0]  x,x+1/2,1/4  [u,u,0]  x,x+1/2,1/4  [u,u,0] |

8 d ..2 x,x,0  [u,u,0]  x,x,0  [u,u,0]  x,x+1/2,1/4  [u,u,0]  x,x+1/2,1/4  [u,u,0] |

8 c 2.. 0,0,z  [0,0,w]  0,0,z  [0,0,w]  0,1/2,z+1/4  [0,0,w]  0,1/2,z+1/4  [0,0,w] |

4 b 2.22 0,0,1/2  [0,0,0]  0,1/2,3/4  [0,0,0] |

4 a 2.22 0,0,0  [0,0,0]  0,1/2,1/4  [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4mm
a* = (a - b)/2  b* = (a + b)/2
Origin at 1/4,1/4,z

Along [1,0,0] c2m'm'
a* = b  b* = c
Origin at x,0,3/8

Along [1,1,0] p2m'm'
a* = -(a + b)/2  b* = c/2
Origin at x,x,0
Origin at 2221' at 2121'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0)$ + set

1. 1
   (0,0,0)

2. $2 \cdot 0,0,z$
   $(2_z \cdot 0,0,0)$

3. $4^+ (0,0,1/4) -1/4,1/4,z$
   $(4_z \cdot 0,1/2,1/4)$

4. $4^- (0,0,1/4) 1/4,1/4,z$
   $(4_z^{-1} \cdot 0,1/2,1/4)$

5. $2 (0,1/2,0) 0,y,1/8$
   $(2_y \cdot 0,1/2,1/4)$

6. $2 \cdot x,1/4,1/8$
   $(2_x \cdot 0,1/2,1/4)$

7. $2 \cdot x,x,0$
   $(2_{xy} \cdot 0,0,0)$

8. $2 \cdot x,x,0$
   $(2_{xy} \cdot 0,0,0)$

For $(1/2,1/2,1/2)$ + set

1. $t (1/2,1/2,1/2)$
   $(1 \cdot 1/2,1/2,1/2)$

2. $2 \cdot (0,0,1/2) 1/4,1/4,z$
   $(2_x \cdot 1/2,1/2,1/2)$

3. $4^+ (0,0,3/4) 1/4,1/4,z$
   $(4_z \cdot 1/2,0,3/4)$

4. $4^- (0,0,3/4) 1/4,-1/4,z$
   $(4_z^{-1} \cdot 1/2,0,3/4)$

5. $2 \cdot 1/4,y,3/8$
   $(2_y \cdot 1/2,0,3/4)$

6. $2 \cdot (1/2,0,0) x,0,3/8$
   $(2_x \cdot 1/2,0,3/4)$

7. $2 \cdot (1/2,1/2,0) x,x,1/4$
   $(2_{xy} \cdot 1/2,1/2,1/2)$

8. $2 \cdot x,\bar{x},+1/2,1/4$
   $(2_{xy} \cdot 1/2,1/2,1/2)$
Continued

For (0,0,0)' + set

(1) 1' (1 0,0,0)'
(2) 2' 0,0,z
(2z 0,0,0)'
(3) 4' (0,0,1/4) -1/4,1/4,z
(4z 0,1/2,1/4)'
(4) 4' (0,0,1/4) 1/4,1/4,z
(4z' 0,1/2,1/4)'

(5) 2' (0,1/2,0) 0,y,1/8
(2y 0,1/2,1/4)'
(6) 2' x,1/4,1/8
(2x 0,1/2,1/4)'
(7) 2' x,x,0
(2xy 0,0,0)'
(8) 2' x,x,0
(2xy' 0,0,0)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)
(1/2,1/2,1/2)'
(2) 2' (0,1/2) 1/4,1/4,z
(2z 1/2,1/2,1/2)'
(3) 4' (0,0,3/4) 1/4,1/4,z
(4z 1/2,0,3/4)'
(4) 4' (0,0,3/4) 1/4,-1/4,z
(4z' 1/2,0,3/4)'

(5) 2' (1/2,0,0) x,0,3/8
(2x 1/2,0,3/4)'
(6) 2' (1/2,1/2,0) x,x,1/4
(2xy 1/2,1/2,1/2)'
(7) 2' (1/2,1/2,0) x,x,1/4
(2xy' 1/2,1/2,1/2)'
(8) 2' x,x+1/2,1/4
(2xy' 1/2,1/2,1/2)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

16 g 11' (1) x,y,z [0,0,0]
(2) x,y,z [0,0,0]
(3) y,x+1/2,z+1/4 [0,0,0]
(4) y,x+1/2,z+1/4 [0,0,0]
(5) x,y+1/2,z+1/4 [0,0,0]
(6) x,y+1/2,z+1/4 [0,0,0]
(7) y,x,z [0,0,0]
(8) y,x,z [0,0,0]

8 f .2.1' x,1/4,1/8 [0,0,0]
(2) x,3/4,1/8 [0,0,0]
(3) 1/4,x,7/8 [0,0,0]
(4) 3/4,x,7/8 [0,0,0]

8 e ..21' x,x,0 [0,0,0]
(2) x,x,0 [0,0,0]
(3) x,x+1/2,1/4 [0,0,0]
(4) x,x+1/2,1/4 [0,0,0]

8 d ..21' x,x,0 [0,0,0]
(2) x,x,0 [0,0,0]
(3) x,x+1/2,1/4 [0,0,0]
(4) x,x+1/2,1/4 [0,0,0]

8 c 2..1' 0,0,z [0,0,0]
(2) 0,0,z [0,0,0]
(3) 0,1/2,z+1/4 [0,0,0]
(4) 0,1/2,z+1/4 [0,0,0]

4 b 2.221' 0,0,1/2 [0,0,0]
(2) 0,1/2,3/4 [0,0,0]
(3) 0,1/2,3/4 [0,0,0]

4 a 2.221' 0,0,0 [0,0,0]
(2) 0,1/2,1/4 [0,0,0]
(3) 0,1/2,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  
Along [1,0,0] c2mm1'  
Along [1,1,0] p2mm1'  

\[ a^* = \frac{(a - b)}{2} \]
\[ b^* = \frac{(a + b)}{2} \]

Origin at 1/4,1/4,z

\[ a^* = b \quad b^* = c \]

Origin at x,0,3/8

\[ a^* = \frac{-(a + b)}{2} \quad b^* = c/2 \]

Origin at x,x,0
I4₁,2₂’
98.3.816

Tetragonal

Origin at 2₂’₂’ at 2₁₂’

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

For (0,0,0) + set

1
(1) 1
(1 | 0,0,0)

2
(2) 0,0,z
(2 | 0,0,0)

4
(3) 4⁺ (0,0,1/4) -1/4,1/4,z
(4 | 0,1/2,1/4)⁺

4⁻⁻ (0,0,1/4) 1/4,1/4,z
(4⁻⁻ | 0,1/2,1/4)⁻⁻

For (1/2,1/2,1/2) + set

1
(1) t (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)

2
(2) 0,0,1/2
(2 | 1/2,1/2,1/2)

4
(3) 4⁺⁺ (0,0,3/4) 1/4,1/4,z
(4 | 1/2,0,3/4)⁺⁺

4⁻⁻ (0,0,3/4) 1/4,-1/4,z
(4⁻⁻ | 1/2,0,3/4)⁻⁻

For (1/2,1/2,1/2) + set

2
(5) 1/4,y,3/8
(2 | 1/2,0,3/4)

2
(6) 1/2,0,0
(2 | 1/2,0,3/4)

4
(7) 2’ (1/2,1/2,0) x,x,1/4
(2 | 1/2,1/2,1/2)’

4⁻⁻ (0,0,1/4) 1/4,1/4,z
(4⁻⁻ | 1/2,0,3/4)⁻⁻

For (1/2,1/2,1/2) + set

2
(8) x,x +1/2,1/4
(2 | 1/2,1/2,1/2)’
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y, z [u,v,w]</td>
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<tr>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
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<tr>
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<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
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<td>8 f .2. x,1/4,1/8 [u,0,0]</td>
<td>x,3/4,1/8 [u,0,0]</td>
</tr>
<tr>
<td>8 e .2' x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
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<tr>
<td>8 d .2' x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
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<tr>
<td>8 c 2. 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<td>4 b 2.2' 0,0,1/2 [0,0,w]</td>
<td>0,1/2,3/4 [0,0,w]</td>
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<tr>
<td>4 a 2.2' 0,0,0 [0,0,w]</td>
<td>0,1/2,1/4 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4m'm' Along [1,0,0] c2m'm' Along [1,1,0] p2mm'
a* = (a - b)/2 b* = (a + b)/2 a* = b b* = c a* = -c/2 b* = (-a + b)/2
Origin at 1/4,1/4,z Origin at x,0,3/8 Origin at x,x,0

98.3.816 - 2 - 1626
I4₁,2'2' 
98.4.817

42'2' 
I4₁,2'2'

Tetragonal

Origin at 22'2' at 212'

Asymmetric unit 
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

For (0,0,0) + set

(1) 1 
(1 0,0,0) 

(2) 2 0,0,z 
(2z 0,0,0) 

(3) 4⁺ (0,0,1/4) -1/4,1/4,z 
(4z 0,1/2,1/4) 

(4) 4⁻ (0,0,1/4) 1/4,1/4,z 
(4z⁻¹ 0,1/2,1/4)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) 
(1 1/2,1/2,1/2) 

(2) 2 (0,0,1/2) 1/4,1/4,z 
(2z 1/2,1/2,1/2) 

(3) 4⁺ (0,0,3/4) 1/4,1/4,z 
(4z 1/2,0,3/4) 

(4) 4⁻ (0,0,3/4) 1/4,-1/4,z 
(4z⁻¹ 1/2,0,3/4)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) 
(1 1/2,1/2,1/2) 

(2) 2 (0,0,1/2) 1/4,1/4,z 
(2z 1/2,1/2,1/2) 

(3) 4⁺ (0,0,3/4) 1/4,1/4,z 
(4z 1/2,0,3/4) 

(4) 4⁻ (0,0,3/4) 1/4,-1/4,z 
(4z⁻¹ 1/2,0,3/4)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<tr>
<th>Positions</th>
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<th>Coordinates</th>
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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(2) ( \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}] )</td>
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<tr>
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<td></td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
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<td></td>
<td>(4) ( y, x+1/2, z+1/4 [v, \bar{u}, \bar{w}] )</td>
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<td>(5) x,y+1/2,( \bar{z} +1/4 [u, \bar{v}, \bar{w}] )</td>
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<td></td>
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<td>(6) x,( y+1/2, \bar{z} +1/4 [u, v, w] )</td>
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<td>(7) y,x,( \bar{z} [v, u, w] )</td>
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<tr>
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<td>(8) ( \bar{y}, x, z [v, u, w] )</td>
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<td>8 f</td>
<td>.2'</td>
<td>x,1/4,1/8 [0,v,w]</td>
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<td>1/4,x,7/8 [( \bar{v}, 0, w )]</td>
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<td>3/4,x,7/8 [v,0,w]</td>
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<td>.2'</td>
<td>x,x,0 [u,u,w]</td>
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<td>x,x,0 [( u, \bar{v}, u, w )]</td>
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<td>8 d</td>
<td>.2'</td>
<td>x,x,0 [( u, u, w )]</td>
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<td>x,x,0 [( u, \bar{u}, w )]</td>
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<td>2.2'</td>
<td>0,0,1/2 [0,0,w]</td>
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<td>0,1/2,3/4 [0,0,w]</td>
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</table>

Symmetry of Special Projections

- Along [0,0,1] p4m'm'
  - \( a^* = (a - b)/2 \)
  - \( b^* = (a + b)/2 \)
- Origin at 1/4,1/4,z

- Along [1,0,0] c2m'm'
  - \( a^* = -c \)
- Origin at x,0,3/8

- Along [1,1,0] p2mm'
  - \( a^* = -c/2 \)
  - \( b^* = (-a + b)/2 \)
- Origin at x,x,0
Origin at 222 at 212

Asymmetric unit: \(0 \leq x \leq 1/2;\) \(0 \leq y \leq 1;\) \(0 \leq z \leq 1/8\)

Symmetry Operations

For \((0,0,0)\) + set

1. \((1,0,0,0)\)
2. \((2,0,0,z)\) \((2_z,0,0,0)\)
3. \((4^+, (0,0,1/4), -1/4,1/4,z)\) \((4_z,0,1/2,1/4)\)
4. \((4^-, (0,0,1/4), 1/4,1/4,z)\) \((4_z^{-1},0,1/2,1/4)\)
5. \((2', (0,1/2,0), 0,y,1/8)\) \((2_z',0,1/2,1/4)\)
6. \((2', x,1/4,1/8)\) \((2_z',0,1/2,1/4)\)
7. \((2, x,x,0)\) \((2_x,0,0,0)\)
8. \((2, x,x,0)\) \((2_x,0,0,0)\)

For \((1/2,1/2,1/2)\) + set

1. \((1/2,1/2,1/2)\)
2. \((2, (0,0,1/2), 1/4,1/4,z)\) \((2_z,1/2,1/2,1/2)\)
3. \((4^+, (0,0,3/4), 1/4,1/4,z)\) \((4_z,1/2,0,3/4)\)
4. \((4^-, (0,0,3/4), 1/4,-1/4,z)\) \((4_z^{-1},1/2,0,3/4)\)
5. \((2', 1/4,y,3/8)\) \((2_z',1/2,0,3/4)\)
6. \((2', (1/2,0,0), x,0,3/8)\) \((2_z',1/2,0,3/4)\)
7. \((2, (1/2,1/2,0), x,x,1/4)\) \((2_x,1/2,1/2,1/2)\)
8. \((2, x,x+1/2,1/4)\) \((2_x,1/2,1/2,1/2)\)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

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<tr>
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<td>0,0,0 [0,0,0]</td>
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**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [1,1,0]</th>
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<tbody>
<tr>
<td>p4'm'm</td>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>a* = (a - b)/2</td>
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<tr>
<td>c2'm'm'</td>
<td>a* = -c</td>
<td>b* = b</td>
<td>a* = -c</td>
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<tr>
<td>p2m'm'</td>
<td>a* = -(a + b)/2</td>
<td>b* = c/2</td>
<td>a* = -(a + b)/2</td>
</tr>
</tbody>
</table>

Origin at 1/4,1/4,z

Origin at x,0,3/8

Origin at x,x,0
### Symmetry Operations

**For (0,0,0) + set**

1. $I$, $(0,0,0)$
2. $2', (0,0,0)$
3. $4^*, (0,0,1/4)$
4. $4^* (0,0,1/4)$
5. $2' (0,1/2,0)$
6. $2 x, 1/4, 1/8$
7. $2', x, x, 0$
8. $2 x, x, 0$

**For $(1/2,1/2,1/2)' + set**

1. $t' (1/2,1/2,1/2)$
2. $2 (0,0,1/2)$
3. $4^* (0,0,3/4)$
4. $4^* (0,0,3/4)$
5. $2 (1/2,0,0)$
6. $2' (1/2,0,0)$
7. $2 (1/2,1/2,0)$
8. $2' x, x + 1/2, 1/4$

### Origin

At $2'2'2$ at $2'1(2',2)$

### Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>16 g 1</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p_c; 4mm
a* = (a - b)/2
b* = (a + b)/2
Origin at 1/4,-1/4,z

Along [1,0,0] c_p; 2mm'
a* = b
b* = c
Origin at x,0,3/8

Along [1,1,0] p_2x; 2mm
a* = -c/2
b* = (-a + b)/2
Origin at x,x,1/4
Origin at $2'22'$ at $2'1(2,2')$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) + \text{set}$

1. $(1) \quad 1$
   
   \begin{align*}
   (1 | 0,0,0)
   \end{align*}

2. $(2) \quad 2' \quad 0,0,z$
   
   \begin{align*}
   (2_1 | 0,0,0)'
   \end{align*}

3. $(3) \quad 4^* \cdot (0,0,1/4) \quad -1/4,1/4,z$
   
   \begin{align*}
   (4_1 | 0,1/2,1/4)'
   \end{align*}

4. $(4) \quad 4^* \cdot (0,0,1/4) \quad 1/4,1/4,z$
   
   \begin{align*}
   (4_1^{-1} | 0,1/2,1/4)
   \end{align*}

5. $(5) \quad 2' \quad (0,1/2,0) \quad 0,y,1/8$
   
   \begin{align*}
   (2_1 | 0,1/2,1/4)'
   \end{align*}

6. $(6) \quad 2 \quad x,1/4,1/8$
   
   \begin{align*}
   (2_1 | 0,1/2,1/4)
   \end{align*}

7. $(7) \quad 2 \quad x,x,0$
   
   \begin{align*}
   (2_{xy} | 0,0,0)
   \end{align*}

8. $(8) \quad 2' \quad x,x,0$
   
   \begin{align*}
   (2_{xy}^{-1} | 0,0,0)'
   \end{align*}

For $(1/2,1/2,1/2') + \text{set}$

1. $(1) \quad t' \quad (1/2,1/2,1/2)$
   
   \begin{align*}
   (1 | 1/2,1/2,1/2)'
   \end{align*}

2. $(2) \quad 2 \quad (0,0,1/2) \quad 1/4,1/4,z$
   
   \begin{align*}
   (2_1 | 1/2,1/2,1/2)
   \end{align*}

3. $(3) \quad 4^* \cdot (0,0,3/4) \quad 1/4,1/4,z$
   
   \begin{align*}
   (4_1 | 1/2,0,3/4)
   \end{align*}

4. $(4) \quad 4^* \cdot (0,0,3/4) \quad 1/4,-1/4,z$
   
   \begin{align*}
   (4_1^{-1} | 1/2,0,3/4)'
   \end{align*}

5. $(5) \quad 2 \quad 1/4,y,3/8$
   
   \begin{align*}
   (2_1 | 1/2,0,3/4)
   \end{align*}

6. $(6) \quad 2' \quad (1/2,0,0) \quad x,0,3/8$
   
   \begin{align*}
   (2_1 | 1/2,0,3/4)'
   \end{align*}

7. $(7) \quad 2' \quad (1/2,1/2,0) \quad x,x,1/4$
   
   \begin{align*}
   (2_{xy} | 1/2,1/2,1/2)'
   \end{align*}

8. $(8) \quad 2 \quad x,x+1/2,1/4$
   
   \begin{align*}
   (2_{xy} | 1/2,1/2,1/2)
   \end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t’(1/2,1/2,1/2); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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Origin at 2'2'2' at 2'1(2,2')

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) +$ set

1. $1 \quad (1|0,0,0)
2. 2' \quad (2|0,0,z)
   \quad (2x|0,0,0)'
3. 4' \quad (0,0,1/4) \quad -1/4,1/4,z
   \quad (4z|0,1/2,1/4)
4. 4' \quad (0,0,1/4) \quad 1/4,1/4,z
   \quad (4z^{-1}|0,1/2,1/4)'
5. 2 \quad (0,1/2,0) \quad 0,y,1/8
   \quad (2x|0,1/2,1/4)'
6. 2' \quad x,1/4,1/8
   \quad (2x|0,1/2,1/4)'
7. 2 \quad x,x,0
   \quad (2x|0,0,0)
8. 2' \quad x,x,0
   \quad (2x|0,0,0)'

For $(1/2,1/2,1/2)' +$ set

1. $t' \quad (1/2,1/2,1/2) \quad (1|1/2,1/2,1/2)'
2. 2 (0,0,1/2) \quad 1/4,1/4,z
   \quad (2z|1/2,1/2,1/2)
3. 4' \quad (0,0,3/4) \quad 1/4,1/4,z
   \quad (4z|1/2,0,3/4)'
4. 4' \quad (0,0,3/4) \quad 1/4,-1/4,z
   \quad (4z^{-1}|1/2,0,3/4)
5. 2' \quad 1/4,y,3/8
   \quad (2z|1/2,0,3/4)'
6. 2 (1/2,0,0) \quad x,0,3/8
   \quad (2z|1/2,0,3/4)
7. 2' \quad (1/2,1/2,0) \quad x,x,1/4
   \quad (2xy|1/2,1/2,1/2)'
8. 2 \quad x,\bar{x}+1/2,1/4
   \quad (2x|1/2,1/2,1/2)
Generators selected
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| 8            | f .2'          | x,1/4,1/8 [0,v,w] |
|              |                | x,3/4,1/8 [0,v,w] |
|              |                | 1/4,x,7/8 [v,0,w] |
|              |                | 3/4,x,7/8 [v,0,w] |
| 8            | e ..2'         | x,x,0 [u,u,w] |
|              |                | x,x,0 [u,u,w] |
|              |                | x,x+1/2,1/4 [u,u,w] |
|              |                | x,x+1/2,1/4 [u,u,w] |
| 8            | d ..2          | x,x,0 [u,u,0] |
|              |                | x,x,0 [u,u,0] |
|              |                | x,x+1/2,1/4 [u,u,0] |
|              |                | x,x+1/2,1/4 [u,u,0] |
| 8            | c 2'..         | 0,0,z [u,v,0] |
|              |                | 0,0,z [v,u,0] |
|              |                | 0,1/2,z+1/4 [v,u,0] |
|              |                | 0,1/2,z+1/4 [v,u,0] |
| 4            | b 2'.22'       | 0,0,1/2 [u,u,0] |
|              |                | 0,1/2,3/4 [u,u,0] |
| 4            | a 2'.22'       | 0,0,0 [u,u,0] |
|              |                | 0,1/2,1/4 [u,u,0] |

Symmetry of Special Projections

Along [0,0,1]  p\textsubscript{c}, 4m\textsuperscript{m}m'  
\textbf{a}' = (a - b)/2  \textbf{b}' = (a + b)/2  
Origin at 1/4,-1/4,z

Along [1,0,0]  c\textsubscript{p}, 2mm  
\textbf{a}' = -c  \textbf{b}' = b  
Origin at x,0,3/8

Along [1,1,0]  p\textsubscript{2x}, 2mm  
\textbf{a}' = -c/2  \textbf{b}' = (-a + b)/2  
Origin at x,x,0
Origin at 2'2'2 at 2'1(2',2)

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8 \]

Symmetry Operations

For \((0,0,0) +\) set

1. \(1\)
   \(1; 0,0,0\)

2. \(2'\)
   \((2z; 0,0,0)'\)

5. \(2\) \((0,1/2,0)\)
   \(0, y^{1/8}\)
   \((2y; 0,1/2,1/4)\)

For \((1/2,1/2,1/2)' +\) set

1. \(t\) \((1/2,1/2,1/2)\)
   \((1; 1/2,1/2,1/2)'\)

5. \(2'\) \(1/4,y,3/8\)
   \((2y; 1/2,0,3/4)'\)

\(l_p 4', 2'2\)

\[ 98.9.822 \]

4221'

\[ 98.9.822 \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>(8) y,x,z [v,u,w]</td>
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<td>x,1/4,1/8 [0,v,w]</td>
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<td>1/4,x,7/8 [v,0,w]</td>
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<td>x,x,0 [u,u,0]</td>
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<td>x,x+1/2,1/4 [u,u,0]</td>
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<tr>
<td>8 c .2'</td>
<td>0,0,z [u,v,0]</td>
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<td>0,1/2,z+1/4 [v,u,0]</td>
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<td>0,1/2,z+1/4 [v,u,0]</td>
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<tr>
<td>4 b 2'.2'2</td>
<td>0,0,1/2 [u,u,0]</td>
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<td>0,1/2,3/4 [u,u,0]</td>
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<tr>
<td>4 a 2'.2'2</td>
<td>0,0,0 [u,u,0]</td>
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<td>0,1/2,1/4 [u,u,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_b, 4mm
a* = (a - b)/2 b* = (a + b)/2
Origin at 1/4,1/4,z

Along [1,0,0] c_p, 2mm'
a* = b b* = c
Origin at x,0,3/8

Along [1,1,0] p_{2x}, 2mm
a* = -c/2 b* = (-a + b)/2
Origin at x,x,0
**Origin** on 4mm

**Asymmetric unit**

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1; \quad x \leq y \]

**Symmetry Operations**

1. \( 1 \)  (1|0,0,0)
2. \( 2 \) 0,0,z  (2|z|0,0,0)
3. \( 4^+ \) 0,0,z  (4|z|0,0,0)
4. \( 4^- \) 0,0,z  (4|z|0,0,0)
5. \( m \)  x,0,z  (m|x|0,0,0)
6. \( m \) 0,y,z  (m|y|0,0,0)
7. \( m \) x,x,z  (m|x|0,y,0)
8. \( m \) x,x,z  (m|x|0,y,0)

**Tetragonal**

P4mm  

|99.1.823| 4mm  
P4mm  

273x38 99.1.823 - 1 - 1639
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<th>Coordinates</th>
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<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(7) y,x,z [v,u,w]</td>
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<td>x,1/2,z [0,v,0]</td>
<td>1/2,x,z [v,0,0]</td>
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<tr>
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<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
<td>0,x,z [v,0,0]</td>
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<tr>
<td>4</td>
<td>d .m</td>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
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<td>2</td>
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<td>0,1/2,z [0,0,0]</td>
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<tr>
<td>1</td>
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<tr>
<td>1</td>
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Symmetry of Special Projections

Along [0,0,1]  p4mm  

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<tr>
<th>a* = a</th>
<th>b* = b</th>
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Origin at 0,0,z

Along [1,0,0]  p1m11'  

<table>
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<th>a* = b</th>
<th>b* = c</th>
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Origin at x,0,0

Along [1,1,0]  p1m11'  

<table>
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<tr>
<th>a* = (-a + b)/2</th>
<th>b* = c</th>
</tr>
</thead>
</table>

Origin at x,x,0

99.1.823 - 2 - 1640
Origin on 4mm1'

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x < y \]

Symmetry Operations

For 1 + set

1. \( (1)\ 1 \)
2. \( (2)\ 2\ 0,0,z \)
3. \( (3)\ 4^+\ 0,0,z \)
4. \( (4)\ 4^+\ 0,0,z \)

(1) \( (1 \ 0,0,0) \)
(2) \( (2 \ 0,0,0') \)
(3) \( (3 \ 0,0,0') \)
(4) \( (4 \ 0,0,0') \)

(5) \( m\ x,0,z \)
(5) \( m\ x,0,0 \)
(7) \( m\ x,0,z \)
(7) \( m\ x,0,0 \)

For 1' + set

1. \( (1')\ 1' \)
2. \( (2')\ 2'\ 0,0,z \)
3. \( (3')\ 4'^+\ 0,0,z \)
4. \( (4')\ 4'^+\ 0,0,z \)

(1) \( (1' \ 0,0,0') \)
(2) \( (2' \ 0,0,0') \)
(3) \( (3' \ 0,0,0') \)
(4) \( (4' \ 0,0,0') \)

(5) \( m'\ x,0,z \)
(5) \( m'\ x,0,0 \)
(7) \( m'\ x,0,z \)
(7) \( m'\ x,0,0 \)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

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<th>Coordinates</th>
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<td>(7) y̅,x̅,z [0,0,0]</td>
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<td>(8) y̅,x̅,z [0,0,0]</td>
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<tr>
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<td>(4) x,1/2,z [0,0,0]</td>
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<td>1/2,x,z [0,0,0]</td>
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<td>1/2,x,z [0,0,0]</td>
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<tr>
<td>4 e .m.1'</td>
<td>(5) x,0,z [0,0,0]</td>
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<td>x,0,z [0,0,0]</td>
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<tr>
<td>x,0,z [0,0,0]</td>
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<tr>
<td>0,x,z [0,0,0]</td>
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<tr>
<td>0,x,z [0,0,0]</td>
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</tr>
<tr>
<td>4 d ..m1'</td>
<td>(6) x,x,z [0,0,0]</td>
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<td>x,x,z [0,0,0]</td>
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<tr>
<td>x,x,z [0,0,0]</td>
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<tr>
<td>x,x,z [0,0,0]</td>
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<tr>
<td>2 c 2mm.1'</td>
<td>(7) 0,1/2,z [0,0,0]</td>
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<td>1/2,0,z [0,0,0]</td>
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<td>1/2,0,z [0,0,0]</td>
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<tr>
<td>1 b 4mm1'</td>
<td>(8) 0,0,z [0,0,0]</td>
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<tr>
<td>1 a 4mm1'</td>
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<tr>
<td>0,0,z [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1'</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [1,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a   b* = b</td>
<td>a* = b   b* = c</td>
<td>a* = (-a + b)/2   b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 4'm'm

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1; \quad x \leq y \]

Symmetry Operations

1. \( 1 \)
   
   \[
   (1|0,0,0)
   \]

2. \( 2 \quad 0,0,z \)
   
   \[
   (2_z|0,0,0)
   \]

3. \( 4^+ \quad 0,0,z \)
   
   \[
   (4_z|0,0,0)'
   \]

4. \( 4^- \quad 0,0,z \)
   
   \[
   (4_z^{-1}|0,0,0)'
   \]

5. \( m' \quad x,0,z \)
   
   \[
   (m_x|0,0,0)'
   \]

6. \( m' \quad y,0,z \)
   
   \[
   (m_y|0,0,0)'
   \]

7. \( m \quad x,x,z \)
   
   \[
   (m_x|0,0,0)
   \]

8. \( m \quad x,x,z \)
   
   \[
   (m_y|0,0,0)
   \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<tr>
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<td>f .m'</td>
<td>x,1/2,z [u,0,w]</td>
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<tr>
<td>1</td>
<td>a 4'm'm</td>
<td>0,0,z [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4'm'm</th>
<th>Along [1,0,0] p1m1'</th>
<th>Along [1,1,0] p1m11'</th>
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</thead>
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<tr>
<td>a* = a b* = b</td>
<td>a* = b b* = c</td>
<td>a* = (-a + b)/2 b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 4'\text{mm}'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\)

Symmetry Operations

\begin{align*}
(1) \quad & \begin{array}{c} 1 \\ (1|0,0,0) \end{array} \\
(2) \quad & \begin{array}{c} 2 \ 0,0,z \\ (2_z|0,0,0) \end{array} \\
(3) \quad & \begin{array}{c} 4'\times \ 0,0,z \\ (4_z|0,0,0)' \end{array} \\
(4) \quad & \begin{array}{c} 4' \times \ 0,0,z \\ (4_z^{-1}|0,0,0)' \end{array} \\
(5) \quad & \begin{array}{c} m \ x,0,z \\ (m_y|0,0,0) \end{array} \\
(6) \quad & \begin{array}{c} m \ 0,y,z \\ (m_x|0,0,0) \end{array} \\
(7) \quad & \begin{array}{c} m' \ x,x,z \\ (m_{xy}|0,0,0)' \end{array} \\
(8) \quad & \begin{array}{c} m' \ x,x,z \\ (m_{xy}|0,0,0)' \end{array}
\end{align*}
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>x,1/2,z [0,v,0]</td>
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<tr>
<td>4 e .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>4 d .m'</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>2 c 2mm.</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>1 b 4'mm'</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>1 a 4'mm'</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'mm'  
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p1m11'  
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p1m1'  
\[ a^* = (-a+b)/2 \quad b^* = c \]
Origin at x,x,0
Origin on 4m' m'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\)

Symmetry Operations

1. \(1\)
   - \((0,0,0)\)
2. \(2\)
   - \((0,0,z)\)
   - \((2z,0,0)\)
3. \(4^+\)
   - \((0,0,z)\)
   - \((4z,0,0)\)
4. \(4^-\)
   - \((0,0,z)\)
   - \((4z^-1,0,0)\)
5. \(m'\)
   - \((x,0,z)\)
   - \((m_y,0,0)\)'
6. \(m'\)
   - \((0,y,z)\)
   - \((m_x,0,0)\)'
7. \(m'\)
   - \((x,x,z)\)
   - \((m_{xy},0,0)\)'
8. \(m'\)
   - \((x,x,z)\)
   - \((m_{xy},0,0)\)'

P4m' m'

99.5.827

Tetragonal

P4m' m'
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tr>
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<td>4 f m'</td>
<td>1</td>
<td>x, 1/2, z [u, 0, w]</td>
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<td>4 e m'</td>
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<td>x, 0, z [u, 0, w]</td>
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<tr>
<td>4 d m'</td>
<td>1</td>
<td>x, x, z [u, u, w]</td>
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<tr>
<td>2 c m'</td>
<td>1</td>
<td>1/2, 0, z [0, 0, w]</td>
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<tr>
<td>1 b m'</td>
<td>1</td>
<td>1/2, 1/2, z [0, 0, w]</td>
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<tr>
<td>1 a m'</td>
<td>1</td>
<td>0, 0, z [0, 0, w]</td>
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Symmetry of Special Projections

Along [0,0,1] p4m' m'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
Origin at 0,0,z

Along [1,0,0] p1m'  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)
Origin at x,0,0

Along [1,1,0] p1m'  
\( \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \)
Origin at x,x,0
### Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
2. \(2\) 0,0,z
3. \(4^+\) 0,0,z
4. \(4^-\) 0,0,z
5. \(m\) x,0,z
6. \(m\) 0,y,z
7. \(m\) x,x,z
8. \(m\) x,x,z

For \((0,0,1)\) + set

1. \(t\) (0,0,1)
2. \(2^\prime\) (0,0,1) 0,0,z
3. \(4^+\) (0,0,1) 0,0,z
4. \(4^-\) (0,0,1) 0,0,z
5. \(c\) (0,0,1) x,0,z
6. \(c^\prime\) (0,0,1) 0,y,z
7. \(c\) (0,0,1) x,x,z
8. \(c^\prime\) (0,0,1) x,x,z

**Origin** on 4mm

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\]
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>.m.</td>
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<td>x,x,z [u,u,0]</td>
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<td>a</td>
<td>4mm</td>
<td>0,0,z [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1] p4mm1'  
Along [1,0,0] p1m11'  
Along [1,1,0] p1m11'

\[ a^* = a \quad b^* = b \]
\[ a^* = b \quad b^* = c \]
\[ a^* = (a + b)/2 \quad b^* = c \]

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0
Origin on 4mm

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1; \quad x \leq y \]

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
   \(1\) \(0,0,0\)
2. \(2 \times 0,0,z\)
   \(2_{z} \times 0,0,0\)
3. \(4^* \times 0,0,z\)
   \(4_{z} \times 0,0,0\)
4. \(4^* \times 0,0,z\)
   \(4_{z}^{-1} \times 0,0,0\)
5. \(m \times x,0,z\)
   \(m_{y} \times 0,0,0\)
6. \(m \times y,0,z\)
   \(m_{x} \times 0,0,0\)
7. \(m \times x,0,z\)
   \(m_{x} \times 0,0,0\)
8. \(m \times x,z\)
   \(m_{x} \times 0,0,0\)

For \((1,0,0)' + set\)

1. \(t'(1,0,0)\)
   \(1_{1} \times 1,0,0\)
2. \(2' \times 1/2,0,z\)
   \(2_{z} \times 1,0,0\)
3. \(4^* ' \times 1/2,1/2,z\)
   \(4_{z} \times 1,0,0\)
4. \(4^* ' \times 1/2,-1/2,z\)
   \(4_{z}^{-1} \times 1,0,0\)
5. \(a'(1,0,0) \times x,0,z\)
   \(m_{y} \times 1,0,0\)
6. \(m' \times 1/2,y,z\)
   \(m_{x} \times 1,0,0\)
7. \(g'(1/2,-1/2,0) \times x+1/2,y,z\)
   \(m_{y} \times 1,0,0\)
8. \(g'(1/2,1/2,0) \times x+1/2,x,z\)
   \(m_{y} \times 1,0,0\)
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>(1,0,0)' +</td>
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<td>4',0,z [0,0,0]</td>
</tr>
<tr>
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<td>4mm</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p₁m₁1' a* = a b* = b
Origin at 0,0,z

Along [1,0,0] p₁m₁1' a* = b b* = c
Origin at x,0,0

Along [1,1,0] p₁m₁1' a* = (-a + b)/2 b* = c
Origin at x,x,0

Pₚ, 4mm
Origin on 4mm

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\)

Symmetry Operations

For \((0,0,0)\) + set

\((1) 1 \quad (2) 2 \quad (3) 4^* \quad (4) 4^*\)

\((1) 0,0,0 \quad (2) 0,0,z \quad (3) 0,0,0 \quad (4) 0,0,0\)

\((5) m \quad (6) m \quad (7) m \quad (8) m\)

\((5) x,0,z \quad (6) 0,y,z \quad (7) x,x,z \quad (8) x,x,z\)

\((5) (m_x|0,0,0) \quad (6) (m_y|0,0,0) \quad (7) (m_x|0,0,0) \quad (8) (m_y|0,0,0)\)

For \((1,0,0)\)' + set

\((1) t' \quad (2) 2' \quad (3) 4^* \quad (4) 4^*\)

\((1) (1,0,0) \quad (2) 1/2,0,z \quad (3) 1/2,1/2,z \quad (4) 1/2,-1/2,z\)

\((5) a' \quad (6) m' \quad (7) g' \quad (8) g'\)

\((5) x,0,z \quad (6) 1/2,y,z \quad (7) x,x+z \quad (8) x,x+z\)

\((5) (m_y|1,0,0) \quad (6) (m_x|1,0,0) \quad (7) (m_x|1,0,0) \quad (8) (m_x|1,0,0)\)

Generators selected \((1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5)\).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

\(16 \quad g \quad 1 \quad (1) x,y,z \quad [u,v,w] \quad (2) x,y,z \quad [v,u,w] \quad (3) y,x,z \quad [v,u,w] \quad (4) y,x,z \quad [v,u,w]\)

\(8 \quad f \quad .m. \quad x,1/2,z \quad [u,0,w] \quad x,1/2,z \quad [u,0,w] \quad 1/2,x,z \quad [0,u,w] \quad 1/2,x,z \quad [0,u,w]\)

\(8 \quad e \quad .m. \quad x,0,z \quad [0,v,0] \quad x,0,z \quad [v,0,0] \quad 0,x,z \quad [v,0,0] \quad 0,x,z \quad [v,0,0]\)

\(8 \quad d \quad .m. \quad x,x,z \quad [0,0,u] \quad 0,x,z \quad [v,u,0] \quad x,x,z \quad [u,0,0] \quad x,x,z \quad [u,0,0]\)

\(4 \quad c \quad 2'm'm. \quad 1/2,0,z \quad [v,0,0] \quad 0,1/2,z \quad [v,0,0]\)

\(2 \quad b \quad 4'm'm \quad 1/2,1/2,z \quad [0,0,0]\)

\(2 \quad a \quad 4mm \quad 0,0,z \quad [0,0,0]\)

Symmetry of Special Projections

Along \([0,0,1]\) \quad p4mm1' \quad Along \([1,0,0]\) \quad p1m11' \quad Along \([1,1,0]\) \quad p1m11'
a^* = a \quad b^* = b \quad a^* = b \quad b^* = c \quad a^* = (-a + b)/2 \quad b^* = c

Origin at \(0,0,z\) \quad Origin at \(x,0,0\) \quad Origin at \(x,x,0\)
Origin on 4'm'm

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1; \ x \leq y$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
2. $2\ 0,0,z$
3. $4'\ 0,0,z$
4. $4''\ 0,0,z$
5. $m'\ x,0,z$
6. $m'\ 0,y,z$
7. $m\ x,x,z$
8. $m\ x,x,z$

For $(0,0,1)$ + set

1. $t'\ (0,0,1)$
2. $2'\ (0,0,1)\ 0,0,z$
3. $4'\ (0,0,1)\ 0,0,z$
4. $4''\ (0,0,1)\ 0,0,z$
5. $c\ (0,0,1)\ x,0,z$
6. $c\ (0,0,1)\ 0,y,z$
7. $c'\ (0,0,1)\ x,x,z$
8. $c'\ (0,0,1)\ x,x,z$
**Generators selected**

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

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<td>a 4'm'm 0,0,z [0,0,0]</td>
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</table>

**Symmetry of Special Projections**

- **Along [0,0,1]** p4mm1'  
  a* = a  b* = b  
  Origin at 0,0,z

- **Along [1,0,0]** p3b1'm1  
  a* = b  b* = c  
  Origin at x,0,0

- **Along [1,1,0]** p1m11'  
  a* = (-a + b)/2  b* = c  
  Origin at x,x,0
**Origin** on 4'mm'

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

**Symmetry Operations**

For (0,0,0) + set

1. $1$
2. $2' 0,0,z (2z \mid 0,0,0)$
3. $4' 0,0,z (4z \mid 0,0,0)'$
4. $4' 0,0,z (4z^{-1} \mid 0,0,0)'$
5. $m x,0,z (m_y \mid 0,0,0)$
6. $m 0,y,z (m_x \mid 0,0,0)$
7. $m' x,x,z (m_{xy} \mid 0,0,0)'$
8. $m' x,x,z (m_{xy}^{-1} \mid 0,0,0)'$

For (0,0,1) + set

1. $t' (0,0,1)$
2. $2' (0,0,1) 0,0,z (2z \mid 0,0,1)'$
3. $4' (0,0,1) 0,0,z (4z \mid 0,0,1)$
4. $4' (0,0,1) 0,0,z (4z^{-1} \mid 0,0,1)$
5. $c' (0,0,1) x,0,z (m_x \mid 0,0,1)'$
6. $c' (0,0,1) 0,y,z (m_y \mid 0,0,1)'$
7. $c (0,0,1) x,x,z (m_{xy} \mid 0,0,1)$
8. $c (0,0,1) x,x,z (m_{xy}^{-1} \mid 0,0,1)$
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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<td>(0,0,1)' +</td>
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<td>1/2,x,z [v,0,0]</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>e .m. x,0,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x',0,z [0,v,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0,x,z [v,0,0]</td>
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<tr>
<td></td>
<td>0,x,z [v,0,0]</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>d ..m' x,x,z [u,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x',x,z [u',u',w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,w]</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c 2mm. 1/2,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b 4'mm' 1/2,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a 4'mm' 0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p4mm1'
  \( \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \)
- Along [1,0,0] p1m11'
  \( \mathbf{a}^* = \mathbf{b}, \mathbf{b}^* = \mathbf{c} \)
- Along [1,1,0] \( p_{2c} \cdot 1m' \)
  \( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2, \mathbf{b}^* = \mathbf{c} \)

Origin at 0,0,z
Origin at x,0,0
Origin at x,x,0
**Symmetry Operations**

### For $(0,0,0)$ + set

1. $1$
   - $(0,0,0)$
2. $2 \cdot 0,0,z$
   - $(2z,0,0,0)$
3. $4^+ \cdot 0,0,z$
   - $(4z,0,0,0)$
4. $4^- \cdot 0,0,z$
   - $(4z^{-1},0,0,0)$
5. $m' \cdot x,0,z$
   - $(m_y,0,0,0)'$
6. $m' \cdot 0,y,z$
   - $(m_x,0,0,0)'$
7. $m' \cdot x,x,z$
   - $(m_{x+y},0,0,0)'$
8. $m' \cdot x,x,z$
   - $(m_{x+y},0,0,0)'$

### For $(0,0,1)$ + set

1. $t' \cdot (0,0,1)$
   - $(1,0,0,1)'$
2. $2' \cdot (0,0,1)$
   - $(2z,0,0,1)'$
3. $4^+ \cdot (0,0,1)$
   - $(4z,0,0,1)'$
4. $4^- \cdot (0,0,1)$
   - $(4z^{-1},0,0,1)'$
5. $c \cdot (0,0,1)$
   - $(m_y,0,0,1)$
6. $c \cdot (0,0,1)$
   - $(m_x,0,0,1)$
7. $c \cdot (0,0,1)$
   - $(m_{x+y},0,0,1)$
8. $c \cdot (0,0,1)$
   - $(m_{x+y},0,0,1)$
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<td>(3) x,y,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
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<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
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<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
</tbody>
</table>

| f 8.m'       | x,1/2,z [u,0,w] |
|              | x,1/2,z [u,0,w] |
|              | 1/2,x,z [0,u,w] |
|              | 1/2,x,z [0,u,w] |

| e 8.m'       | x,0,z [u,0,w] |
|              | x,0,z [u,0,w] |
|              | 0,x,z [0,u,w] |
|              | 0,x,z [0,u,w] |

| d 8.m'       | x,x,z [u,u,w] |
|              | x,x,z [u,u,w] |
|              | x,x,z [u,u,w] |

| c 4m'4m'     | 1/2,0,z [0,0,w] |
|              | 0,1/2,z [0,0,w] |

| b 4m'4m'     | 1/2,1/2,z [0,0,w] |

| a 4m'4m'     | 0,0,z [0,0,w] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1'</th>
<th>Along [1,0,0] p2b'1m1'</th>
<th>Along [1,1,0] p2b'1m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (a + b)/2</td>
</tr>
<tr>
<td>b* = b</td>
<td>c</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,0,0

Origin at x,x,0
Origin on $4'mm'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1 \\
(2) 2 0,0,z \\
(3) 4+ 0,0,z \\
(4) 4- 0,0,z \\
(5) m x,0,z \\
(6) m 0,y,z \\
(7) m' x,x,z \\
(8) m' x,x,z

For $(1,0,0)' +$ set

(1) t' (1,0,0) \\
(2) 2' 1/2,0,z \\
(3) 4+ 1/2,1/2,z \\
(4) 4- 1/2,-1/2,z \\
(5) a' (1,0,0) x,0,z \\
(6) m' 1/2,y,z \\
(7) g (1/2,-1/2,0) x+1/2,x,z \\
(8) g (1/2,1/2,0) x+1/2,x,z

99.12.834 - 1 - 1661
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)'+</td>
</tr>
<tr>
<td>16</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 f .m'</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>8 e .m</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 d ..m'</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>4 c 2'm'</td>
<td>1/2,0,z [0,v,0]</td>
</tr>
<tr>
<td>2 b 4'm'</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a 4'm'</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] pₚ,4m'm'
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
Origin at 1/2,1/2,z

Along [1,0,0] p1m11'
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \)
Origin at x,0,0

Along [1,1,0] pₚ.1m1
\( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \)
Origin at x-1/4,x+1/4,0
Origin on 4mm

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\]

Symmetry Operations

For \((0,0,0)\) + set

1. \((1,0,0,0)\)
2. \((2) \quad 0,0,z\)
3. \((3) \quad 4^* \quad 0,0,z\)
4. \((4) \quad 4^* \quad 0,0,z\)

For \((1,0,0)\)' + set

1. \((1) \quad (1,0,0,0)\)
2. \((2) \quad 1/2,0,z\)
3. \((3) \quad 4^* \quad 1/2,1/2,z\)
4. \((4) \quad 4^* \quad 1/2,-1/2,z\)

Generators selected

1; \(t'(1,0,0); t'(0,1,0); t'(0,0,1)\); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

\[(0,0,0) + \quad (1,0,0)' +\]

16 \(g\)

1. \((1) \quad x,y,z [u,v,w]\)
2. \((2) \quad x,y,z [u,v,w]\)
3. \((3) \quad x,y,z [u,v,w]\)
4. \((4) \quad x,y,z [u,v,w]\)

8 \(f\)

1. \((5) \quad x,y,z [u,v,w]\)
2. \((6) \quad x,y,z [u,v,w]\)
3. \((7) \quad x,y,z [u,v,w]\)
4. \((8) \quad x,y,z [u,v,w]\)

8 \(e\)

1. \((9) \quad x,0,z [u,0,w]\)
2. \((10) \quad x,0,z [u,0,w]\)
3. \((11) \quad x,0,z [u,0,w]\)
4. \((12) \quad x,0,z [u,0,w]\)

4 \(c\)

1. \((13) \quad 2'mm'. \quad 1/2,0,z [u,0,0]\)
2. \((14) \quad 2'mm'. \quad 1/2,0,z [u,0,0]\)
3. \((15) \quad 2'mm'. \quad 1/2,0,z [u,0,0]\)
4. \((16) \quad 2'mm'. \quad 1/2,0,z [u,0,0]\)

Symmetry of Special Projections

Along \([0,0,1]\) \quad \(P_{4mm1}'\)  \quad Along \([1,0,0]\) \quad \(p1m11'\)  \quad Along \([1,1,0]\) \quad \(p_{1cm1}\)

\(\mathbf{a}^* = \mathbf{a}\) \quad \(\mathbf{b}^* = \mathbf{b}\)  \quad \(\mathbf{a}^* = \mathbf{b}\) \quad \(\mathbf{b}^* = \mathbf{c}\)

Origin at \(0,0,0\)  \quad \text{Origin at} \(x,0,0\)  \quad \text{Origin at} \(-x+1/4,x+1/4,0\)
Origin on 41g

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$; $y \leq 1/2-x$

Symmetry Operations

1. $1$
   - $0,0,0$
   - $1/2,0,0$

2. $2$ $0,0,z$
   - $0,0,0$
   - $2z,0,0$

3. $4^+$ $0,0,z$
   - $0,0,0$
   - $4z,0,0$

4. $4^-$ $0,0,z$
   - $0,0,0$
   - $4^{-1}z,0,0$

5. $a$ $(1/2,0,0)$ $x,1/4,z$
   - $(1/2,0,0)$ $x,1/4,z$
   - $(1/2,1/2,0)$ $m_y,1/2,1/2,z$

6. $b$ $(0,1/2,0)$ $1/4,y,z$
   - $(0,1/2,0)$ $1/4,y,z$
   - $(1/2,1/2,0)$ $m_x,1/2,1/2,z$

7. $m$ $x+1/2,x,z$
   - $x+1/2,x,z$
   - $1/2,1/2,z$

8. $g$ $(1/2,1/2,0)$ $x,x,z$
   - $(1/2,1/2,0)$ $x,x,z$
   - $(1/2,1/2,0)$ $m_{xy},1/2,1/2,z$
Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2): (3): (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
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<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
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<td>4 c .m</td>
<td>x,x+1/2,z [u,u,0]</td>
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<td>x,x+1/2,z [u,u,0]</td>
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<tr>
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<td>x,x+1/2,z [u,u,0]</td>
</tr>
<tr>
<td>2 b 2.mm</td>
<td>1/2,0,z [0,0,0]</td>
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<td>1/2,0,z [0,0,0]</td>
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<tr>
<td>2 a 4..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm

\( a^* = a \quad b^* = b \)

Origin at 0,0,z

Along [1,0,0] \( p_{2a}^{-1}m1 \)

\( a^* = b/2 \quad b^* = c \)

Origin at x,1/4,0

Along [1,1,0] \( p1m11' \)

\( a^* = -(a + b)/2 \quad b^* = c \)

Origin at x,x,0
**P4bm1'**

**4mm1'**

**Tetragonal**

**100.2.837**

**P4bm1'**

**Origin** on 41g1'

**Asymmetric unit**

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x
\]

**Symmetry Operations**

For 1 + set

1. \( \begin{aligned} (1) \ 1 \\
(1) 0,0,0 \end{aligned} \)

2. \( \begin{aligned} (2) \ 0,0,z \\
(2z) 0,0,0 \end{aligned} \)

3. \( \begin{aligned} (3) \ 4^+ \ 0,0,z \\
(4z) 0,0,0 \end{aligned} \)

4. \( \begin{aligned} (4) \ 4^- \ 0,0,z \\
(4z^{-1}) 0,0,0 \end{aligned} \)

5. \( \begin{aligned} (5) \ a \ (1/2,0,0) \\
(m_x, 1/2,1/2,0) \end{aligned} \)

6. \( \begin{aligned} (6) \ b \ (0,1/2,0) \\
(m_x, 1/2,1/2,0) \end{aligned} \)

7. \( \begin{aligned} (7) \ m \ x+1/2, x, z \\
(m_{xy}, 1/2,1/2,0) \end{aligned} \)

8. \( \begin{aligned} (8) \ g \ (1/2,1/2,0) \\
(m_{xy}, 1/2,1/2,0) \end{aligned} \)

For 1' + set

1. \( \begin{aligned} (1) \ 1' \\
(1) 0,0,0' \end{aligned} \)

2. \( \begin{aligned} (2) \ 0,0,z' \\
(2z) 0,0,0' \end{aligned} \)

3. \( \begin{aligned} (3) \ 4^+ \ 0,0,z' \\
(4z) 0,0,0' \end{aligned} \)

4. \( \begin{aligned} (4) \ 4^- \ 0,0,z' \\
(4z^{-1}) 0,0,0' \end{aligned} \)

5. \( \begin{aligned} (5) \ a' \ (1/2,0,0) \\
(m_x, 1/2,1/2,0)' \end{aligned} \)

6. \( \begin{aligned} (6) \ b' \ (0,1/2,0) \\
(m_x, 1/2,1/2,0)' \end{aligned} \)

7. \( \begin{aligned} (7) \ m' \ x+1/2, x, z' \\
(m_{xy}, 1/2,1/2,0)' \end{aligned} \)

8. \( \begin{aligned} (8) \ g' \ (1/2,1/2,0) \\
(m_{xy}, 1/2,1/2,0)' \end{aligned} \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
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<tr>
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<td>(2) (\bar{x},\bar{y},z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) (y,x,z) [0,0,0]</td>
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<tr>
<td></td>
<td>(4) (y,\bar{x},z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) (x+1/2,\bar{y}+1/2,z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(6) (\bar{x}+1/2,y+1/2,z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) (\bar{y}+1/2,\bar{x}+1/2,z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(8) (y+1/2,\bar{x}+1/2,z) [0,0,0]</td>
</tr>
<tr>
<td>4 c ..m1' x,x+1/2,z [0,0,0]</td>
<td>(\bar{x},\bar{x}+1/2,z) [0,0,0]</td>
</tr>
<tr>
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<td>(\bar{x}+1/2,\bar{x},z) [0,0,0]</td>
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<td>(x+1/2,\bar{x},z) [0,0,0]</td>
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<tr>
<td>2 b 2.mm1' 1/2,0,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 a 4..1' 0,0,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4gm1'</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [1,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a) (b^* = b)</td>
<td>(a^* = b/2) (b^* = c)</td>
<td>(a^* = -(a + b)/2) (b^* = c)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 4'1g

Asymmetric unit: \(0 \leq x < \frac{1}{2}; \quad 0 \leq y < \frac{1}{2}; \quad 0 \leq z < 1; \quad y < \frac{1}{2} - x\)

Symmetry Operations

1. \(1\) \(0,0,0\)
2. \(2\) \(0,0,z\) \(2z,0,0\)
3. \(4'\) \(0,0,z\) \(4z,0,0'\)
4. \(4''\) \(0,0,z\) \(4z,0,0'\)
5. \(a'\) \((1/2,0,0)\) \(x,1/4,z\) \((m_y|x/2,1/2,0)'\)
6. \(b'\) \((0,1/2,0)\) \(1/4,y,z\) \((m_x|x/2,1/2,0)'\)
7. \(m\) \(x+1/2,x,z\) \((m_x|x/2,1/2,0)\)
8. \(g\) \((1/2,1/2,0)\) \(x,x,z\) \((m_x|x/2,1/2,0)\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8</td>
<td>d 1</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>c m</td>
</tr>
<tr>
<td></td>
<td>x,x+1/2,z [u,u,0]</td>
</tr>
<tr>
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<td>x,x+1/2,z [u,u,0]</td>
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</tr>
<tr>
<td></td>
<td>x,x+1/2,z [u,u,0]</td>
</tr>
<tr>
<td>2</td>
<td>b 2.mm</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
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<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 4'..</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
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<td>1/2,1/2,z [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'g'm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
P4’bm’ 4’mm’ Tetragonal

Origin on 4’1g’

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1; \quad y \leq \frac{1}{2} - x \]

Symmetry Operations

1. \((1)\) 1
   
2. \((2)\) 2 0,0,z
   
3. \((3)\) 4’+ 0,0,z
   
4. \((4)\) 4’- 0,0,z

5. \((5)\) a (1/2,0,0) x,1/4,z
   
6. \((6)\) b (0,1/2,0) 1/4,y,z

7. \((7)\) m’ x+1/2,0,0,z
   
8. \((8)\) g’ (1/2,1/2,0) x,x,z
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>d 1</td>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<td></td>
<td></td>
<td></td>
<td>(3) y,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) y,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
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<td></td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
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<td></td>
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<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>c .m'</td>
<td></td>
<td>x+1/2,z [u,u,w]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>x+1/2,z [u,u,w]</td>
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<td>x+1/2,z [u,u,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 2.m'm'</td>
<td></td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a 4'..</td>
<td></td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p4'gm'
  \( a^* = a \quad b^* = b \)
  Origin at 0,0,z

- Along [1,0,0] p2a1m1
  \( a^* = b/2 \quad b^* = c \)
  Origin at x,1/4,0

- Along [1,1,0] p1m1
  \( a^* = (-a + b)/2 \quad b^* = c \)
  Origin at x,x,0
Origin on 41g'

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x$

Symmetry Operations

1. $1$
   (1) 0,0,0
   (2) $z_0,0,0$

2. $2^{+}$
   (1) $z_0,0,0$
   (2) $z_0,0,0$
   (4) $z_0,0,0$

3. $a'$
   (1) $1/2,0,0$
   (6) $1/2,1/2,0$

4. $b'$
   (1) $1/2,0,0$
   (6) $1/2,1/2,0$

5. $m'$
   (1) $1/2,1/2,0$
   (6) $1/2,1/2,0$

6. $g'$
   (1) $1/2,1/2,0$
   (6) $1/2,1/2,0$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<th>Multiplicity</th>
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<tbody>
<tr>
<td>8 d 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w] (6) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
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<td>(7) y+1/2,x+1/2,z [v,u,w] (8) y+1/2,x+1/2,z [v,u,w]</td>
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<tr>
<td>4 c ..m'</td>
<td>x,x+1/2,z [u,u,w] x,x+1/2,z [u,u,w] x+1/2,x,z [u,u,w] x+1/2,x,z [u,u,w]</td>
</tr>
<tr>
<td>2 b 2.m'</td>
<td>1/2,0,z [0,0,w] 0,1/2,z [0,0,w]</td>
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<td>2 a 4..</td>
<td>0,0,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4g'm'</th>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>

Continued
Origin on 41g

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1; y ≤ 1/2-x

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2z 0,0,0)

(3) 4+ 0,0,z
(4z 0,0,0)

(4) 4- 0,0,z
(4z-1 0,0,0)

(5) a 1/2,0,0 x,1/4,z
(my 1/2,1/2,0)

(6) b (0,1/2,0) 1/4,y,z
(mx 1/2,1/2,0)

(7) m x+1/2,x,z
(mx 1/2,1/2,0)

(8) g (1/2,1/2,0) x,x,z
(my 1/2,1/2,0)

For (0,0,1)' + set

(1) t' (0,0,1)
(1) 0,0,1'

(2) 2' (0,0,1) 0,0,z
(2z 0,0,1')

(3) 4+ ' (0,0,1) 0,0,z
(4z 0,0,1')

(4) 4- ' (0,0,1) 0,0,z
(4z-1 0,0,1')

(5) n' (1/2,0,1) x,1/4,z
(mx 1/2,1/2,1)

(6) n' (0,1/2,1) 1/4,y,z
(mx 1/2,1/2,1')

(7) c' (0,0,1) x+1/2,x,z
(mx 1/2,1/2,1')

(8) n' (1/2,1/2,1) x,x,z
(mx 1/2,1/2,1')
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 d 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
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<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w] (6) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
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<td>(7) y+1/2,x+1/2,z [v,u,w] (8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td>8 c .m</td>
<td>x,x+1/2,z [u,u,0] x,x+1/2,z [u,u,0] x+1/2,x,z [u,u,0] x+1/2,x,z [u,u,0]</td>
</tr>
<tr>
<td>4 b 2.mm</td>
<td>1/2,0,z [0,0,0] 0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 a 4..</td>
<td>0,0,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1’

\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]

Origin at 0,0,z

Along [1,1,0] p1m11’

\[ \mathbf{a}^* = \mathbf{-a} + \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c} \]

Origin at x,x,0

Along [1,0,0] p1m1m1

\[ \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c} \]

Origin at x,1/4,0
Origin on 4’1g

Asymmetric unit: \(0 < x < \frac{1}{2}; \ 0 < y < \frac{1}{2}; \ 0 < z < 1; \ y < \frac{1}{2} - x\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \ (1) \ 0,0,0\)
2. \(2 \ (0,0,z) \ (2z,0,0,0)\)
3. \(4^{+} \ 0,0,z \ (4z,0,0,0)'\)
4. \(4^{-} \ 0,0,z \ (4z^{-1},0,0,0)'\)

5. \(a' \ (1/2,0,0) \ x,1/4,z \ (m_{y},1/2,1/2,0)\)
6. \(b' \ (0,1/2,0) \ 1/4,y,z \ (m_{x},1/2,1/2,0)'\)
7. \(m \ x+1/2,x,z \ (m_{x},1/2,1/2,0)'\)
8. \(g \ (1/2,1/2,0) \ x,x,z \ (m_{y},1/2,1/2,0)'\)

For \((0,0,1)' + \) set

1. \(t' \ (0,0,1) \ (1,0,0,1)\)
2. \(2' \ (0,0,1) \ 0,0,z \ (2z,0,0,1)'\)
3. \(4' \ (0,0,1) \ 0,0,z \ (4z,0,0,1)\)
4. \(4' \ (0,0,1) \ 0,0,z \ (4z^{-1},0,0,1)'\)

5. \(n \ (1/2,0,1) \ x,1/4,z \ (m_{y},1/2,1/2,1)\)
6. \(n \ (0,1/2,1) \ 1/4,y,z \ (m_{x},1/2,1/2,1)'\)
7. \(c' \ (0,0,1) \ x+1/2,x,z \ (m_{y},1/2,1/2,1)'\)
8. \(n' \ (1/2,1/2,1) \ x,x,z \ (m_{y},1/2,1/2,1)'\)
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicities,
Wyckoff letters,
Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' +</td>
<td>(0,0,0)</td>
<td>16</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>d</td>
</tr>
<tr>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1' 
\(a^* = a \quad b^* = b\)
Origin at 0,0,z

Along [1,0,0] p1m1m'1 
\(a^* = b/2 \quad b^* = c\)
Origin at x,0,0

Along [1,1,0] p1m11' 
\(a^* = (-a + b)/2 \quad b^* = c\)
Origin at x,x,0
**Origin** on 4'1g'

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x\]

**Symmetry Operations**

For (0,0,0) + set

1. \(1 \quad 1\)
   \(1 \quad 0,0,0\)
2. \(2 \quad 0,0,z\)
   \(2_z \quad 0,0,0\)
3. \(4^+ \quad 0,0,z\)
   \(4_z \quad 0,0,0\)
4. \(4^- \quad 0,0,z\)
   \(4_z^{-1} \quad 0,0,0\)

5. \(a \quad (1/2,0,0)\)
   \(x,1/4,z\)
   \(m_y \quad 1/2,1/2,0\)

6. \(b \quad (0,1/2,0)\)
   \(1/4,y,z\)
   \(m_x \quad 1/2,1/2,0\)

7. \(m' \quad x+1/2,x,z\)
   \(m_{xy} \quad 1/2,1/2,0\)

8. \(g' \quad (1/2,1/2,0)\)
   \(x,x,z\)
   \(m_{xy} \quad 1/2,1/2,0\)

For (0,0,1)' + set

1. \(t' \quad (0,0,1)\)
   \(1 \quad 0,0,1\)

2. \(2' \quad (0,0,1)\)
   \(0,0,z\)
   \(2_z \quad 0,0,1\)

3. \(4^+ \quad (0,0,1)\)
   \(0,0,z\)
   \(4_z \quad 0,0,1\)

4. \(4^- \quad (0,0,1)\)
   \(0,0,z\)
   \(4_z^{-1} \quad 0,0,1\)

5. \(n' \quad (1/2,0,1)\)
   \(x,1/4,z\)
   \(m_y \quad 1/2,1/2,1\)

6. \(n' \quad (0,1/2,1)\)
   \(1/4,y,z\)
   \(m_x \quad 1/2,1/2,1\)

7. \(c \quad (0,0,1)\)
   \(x+1/2,x,z\)
   \(m_{xy} \quad 1/2,1/2,1\)

8. \(n \quad (1/2,1/2,1)\)
   \(x,x,z\)
   \(m_{xy} \quad 1/2,1/2,1\)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>16 d 1</td>
<td>1</td>
<td>(0,0,0) + (0,0,1) +</td>
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<tr>
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<td></td>
<td>(1) x,y,z [u,v,w]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

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<tr>
<th>Along [0,0,1]</th>
<th>p4gm1'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
</tbody>
</table>

**Along [1,0,0] | p4,1m1**

| a* = b/2     | b* = c |

**Along [1,1,0] | p2c,1m1**

| a* = (-a + b)/2 | b* = c |

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at x,x,0
Origin on 41g'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x\)

Symmetry Operations

For \((0,0,0) + \text{ set}\)

1. \(1\) \(1,0,0,0\)
2. \(2\) \(0,0,z\)\(2_{z},0,0,0\)
3. \(4^{+}\) \(0,0,z\)\(4_{z},0,0,0\)
4. \(4^{-}\) \(0,0,z\)\(4_{z}^{-},0,0,0\)
5. \(a' (1/2,0,0)\) \(x,1/4,z\)\(m_{y}|1/2,1/2,0'\)
6. \(b' (0,1/2,0)\) \(1/4,y,z\)\(m_{x}|1/2,1/2,0'\)
7. \(m' x+1/2,\overline{x},z\)\(m_{x}|1/2,1/2,0'\)
8. \(g' (1/2,1/2,0)\) \(x,x,z\)\(m_{y} | 1/2,1/2,2,0'\)

For \((0,0,1') + \text{ set}\)

1. \(t' (0,0,1)\) \(1,0,0,1'\)
2. \(2' (0,0,1)\) \(0,0,z\)\(2_{z},0,0,1'\)
3. \(4^{+} (0,0,1)\) \(0,0,z\)\(4_{z},0,0,1'\)
4. \(4^{-} (0,0,1)\) \(0,0,z\)\(4_{z}^{-},0,0,1'\)
5. \(n (1/2,0,1)\) \(x,1/4,z\)\(m_{y}|1/2,1/2,0'\)
6. \(n (0,1/2,1)\) \(1/4,y,z\)\(m_{x}|1/2,1/2,1\)
7. \(c (0,0,1)\) \(x+1/2,\overline{x},z\)\(m_{y} | 1/2,1/2,2,1\)
8. \(n (1/2,1/2,1)\) \(x,x,z\)\(m_{y} | 1/2,1/2,2,1\)
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>d 1</td>
<td>(0,0,0) + (0,0,1) +</td>
</tr>
<tr>
<td>16</td>
<td>c ..m'</td>
<td>x,x+1/2,z [u,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>b 2.m'm'</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>a 4..</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p4gm1' \)
\( a^* = a \)  \( b^* = b \)
Origin at 0,0,z

Along [1,0,0] \( p2b.^1m'1 \)
\( a^* = b/2 \)  \( b^* = c \)
Origin at x,0,0

Along [1,1,0] \( p2b.^1m'1 \)
\( a^* = (-a + b)/2 \)  \( b^* = c \)
Origin at x,x,0
**Origin** on 2mm on 4\textsubscript{2} cm

**Asymmetric unit**
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \]

**Symmetry Operations**

1. \(1\)  
   \[
   (1)\, (0,0,0)
   \]

2. \(2\) \(0,0,z\)  
   \[
   (2)\, (z,0,0,0)
   \]

3. \(4^+ (0,0,1/2) 0,0,z\)  
   \[
   (3)\, (4_z,0,0,1/2)
   \]

4. \(4^- (0,0,1/2) 0,0,z\)  
   \[
   (4)\, (4_z^{-1},0,0,1/2)
   \]

5. \(c (0,0,1/2) x,0,z\)  
   \[
   (5)\, (c,0,0,1/2)
   \]

6. \(c (0,0,1/2) 0,y,z\)  
   \[
   (6)\, (c,0,0,1/2)
   \]

7. \(m x,x,z\)  
   \[
   (7)\, (m x,0,0,0)
   \]

8. \(m x,x,z\)  
   \[
   (8)\, (m_x,0,0,0)
   \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>e 1</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>d ..m</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z+1/2 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z+1/2 [u,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>c 2..</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 2.mm</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 2.mm</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Origin at x,0,0</th>
<th>Origin at x,x,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>p4mm</td>
<td>p1m'1</td>
<td>p1m11'</td>
</tr>
<tr>
<td>a* = a</td>
<td>a* = b</td>
<td>a* = (-a + b)/2</td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = c</td>
<td>b* = c</td>
</tr>
</tbody>
</table>
**Symmetry Operations**

For 1 + set

1. $1$  
   $1^{1}$  
   $2$ $0,0,z$  
   $(2_{x}0,0,0)$

5. $c(0,0,1/2)$ $x,0,z$  
   $(m_{y}0,0,1/2)$

6. $c(0,0,1/2)$ $y,0,z$  
   $(m_{x}0,0,1/2)$

7. $m$ $x,x,z$  
   $(m_{xy}0,0,0)$

For $1^{1}$ + set

1. $1^{1}$  
   $(1|0,0,0)^{1}$

2. $2^{1}$ $0,0,z$  
   $(2_{x}0,0,0)^{1}$

5. $c^{1}(0,0,1/2)$ $x,0,z$  
   $(m_{y}0,0,1/2)^{1}$

6. $c^{1}(0,0,1/2)$ $y,0,z$  
   $(m_{x}0,0,1/2)^{1}$

7. $m^{1}$ $x,x,z$  
   $(m_{xy}0,0,0)^{1}$

Origin on 2mm1' on 42 cm1'

Asymmetric unit  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Tetragonal
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 +</td>
<td></td>
</tr>
<tr>
<td>1' +</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>e</th>
<th>11'</th>
<th>(1) x,y,z [0,0,0]</th>
<th>(2) x,y,z [0,0,0]</th>
<th>(3) y,x,z+1/2 [0,0,0]</th>
<th>(4) y,x,z+1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) x,y,z+1/2 [0,0,0]</td>
<td>(6) x,y,z+1/2 [0,0,0]</td>
<td>(7) y,x,z [0,0,0]</td>
<td>(8) y,x,z [0,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>d</th>
<th>..m1'</th>
<th>x,x,z [0,0,0]</th>
<th>x,x,z [0,0,0]</th>
<th>x,x,z+1/2 [0,0,0]</th>
<th>x,x,z+1/2 [0,0,0]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>c</th>
<th>2..1'</th>
<th>0,1/2,z [0,0,0]</th>
<th>1/2,0,z+1/2 [0,0,0]</th>
<th>0,1/2,z+1/2 [0,0,0]</th>
<th>1/2,0,z [0,0,0]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th>b</th>
<th>2.mm1'</th>
<th>1/2,1/2,z [0,0,0]</th>
<th>1/2,1/2,z+1/2 [0,0,0]</th>
<th></th>
<th></th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th>a</th>
<th>2.mm1'</th>
<th>0,0,z+1/2 [0,0,0]</th>
<th>0,0,z+1/2 [0,0,0]</th>
<th></th>
<th></th>
</tr>
</thead>
</table>

### Symmetry of Special Projections

Along [0,0,1] p4mm1'  
*Conclusion of origins in [0,0,0] and [0,0,z]*

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [1,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2mm on $4'_{2}$c'm

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

(1) $1$

(1) $1$

(1) $1$

(1) $1$

(1) $1$

(1) $1$

(1) $1$

(1) $1$

(2) $2 \ 0,0,z$

(2) $2 \ 0,0,z$

(2) $2 \ 0,0,z$

(2) $2 \ 0,0,z$

(2) $2 \ 0,0,z$

(2) $2 \ 0,0,z$

(2) $2 \ 0,0,z$

(2) $2 \ 0,0,z$

(3) $4' \ (0,0,0)$

(3) $4' \ (0,0,0)$

(3) $4' \ (0,0,0)$

(3) $4' \ (0,0,0)$

(3) $4' \ (0,0,0)$

(3) $4' \ (0,0,0)$

(3) $4' \ (0,0,0)$

(3) $4' \ (0,0,0)$

(4) $4' \ (0,0,1/2)$

(4) $4' \ (0,0,1/2)$

(4) $4' \ (0,0,1/2)$

(4) $4' \ (0,0,1/2)$

(4) $4' \ (0,0,1/2)$

(4) $4' \ (0,0,1/2)$

(4) $4' \ (0,0,1/2)$

(4) $4' \ (0,0,1/2)$

(5) $c' \ (0,0,1/2) \ x,0,z$

(5) $c' \ (0,0,1/2) \ x,0,z$

(5) $c' \ (0,0,1/2) \ x,0,z$

(5) $c' \ (0,0,1/2) \ x,0,z$

(5) $c' \ (0,0,1/2) \ x,0,z$

(5) $c' \ (0,0,1/2) \ x,0,z$

(5) $c' \ (0,0,1/2) \ x,0,z$

(5) $c' \ (0,0,1/2) \ x,0,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(6) $c' \ (0,0,1/2) \ 0,y,z$

(7) $m \ x,x.z$

(7) $m \ x,x.z$

(7) $m \ x,x.z$

(7) $m \ x,x.z$

(7) $m \ x,x.z$

(7) $m \ x,x.z$

(7) $m \ x,x.z$

(7) $m \ x,x.z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$

(8) $m \ x,x,z$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

| 8 | e | 1 | (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] | (3) x,x,z+1/2 [v,u,w] | (4) y,x,z+1/2 [v,u,w] |
| 4 | d | m | x,x,z [u,u,0] | x,x,z [u,u,0] | x,x,z+1/2 [u,u,0] | x,x,z+1/2 [u,u,0] |
| 4 | c | 2.. | 0,1/2,z [0,0,0] | 1/2,0,z+1/2 [0,0,w] | 0,1/2,z+1/2 [0,0,w] | 1/2,0,z [0,0,w] |
| 2 | b | 2.mm | 1/2,1/2,z [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] |
| 2 | a | 2.mm | 0,0,z [0,0,0] | 0,0,z+1/2 [0,0,0] | 0,0,z+1/2 [0,0,0] | 0,0,z+1/2 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4' mm1

a* = -b  b* = a

Origin at 0,0,z

Along [1,0,0] p1m'1

a* = b  b* = c/2

Origin at x,0,0

Along [1,1,0] p1m11'

a* = -(a + b)/2  b* = c

Origin at x,x,0
Origin on 2/m’m’ on 4_1 cm’

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\)

Symmetry Operations

1. \((1,0,0,0)\)
2. \(2 \cdot 0,0,z\)
3. \(4^+ \cdot (0,0,1/2) \quad 0,0,z\)
4. \(4^- \cdot (0,0,1/2) \quad 0,0,z\)
5. \(c \cdot (0,0,1/2) \quad x,0,z\)
6. \(c \cdot (0,0,1/2) \quad 0,y,z\)
7. \(m' \cdot x,x,z\)
8. \(m' \cdot x,x,z\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z+1/2 [v,u,w] (4) y,x,z+1/2 [v,u,w] (5) x,y,z+1/2 [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 d ...m'</td>
<td>x,x,z [u,u,w] x,x,z [u,u,w] x,x,z+1/2 [u,u,w] x,x,z+1/2 [u,u,w]</td>
</tr>
<tr>
<td>4 c 2..</td>
<td>0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 0,1/2,z+1/2 [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 b 2.m'm'</td>
<td>1/2,1/2,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 2.m'm'</td>
<td>0,0,z [0,0,w] 0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'mmm' Along [1,0,0] p4m1 Along [1,1,0] p41
a* = a  b* = b  a* = b  b* = c/2  a* = (a + b)/2  b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
Origin on 2m'm' on 42 c'm'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \]

Symmetry Operations

1. \( 1 \)
   \( (1) \) 0,0,0

2. \( 2 \)
   \( (2) \) 0,0,z
   \( (2_z) 0,0,0 \)

3. \( 4^+ \)
   \( (3) \) (0,0,1/2) 0,0,z
   \( (4_z) 0,0,1/2 \)

4. \( 4^- \)
   \( (4) \) (0,0,1/2) 0,0,z
   \( (4_z^-) 0,0,1/2 \)

5. \( c' \)
   \( (5) \) (0,0,1/2) x,0,z
   \( (m_y) 0,0,1/2' \)

6. \( c' \)
   \( (6) \) (0,0,1/2) 0,y,z
   \( (m_x) 0,0,1/2' \)

7. \( m' \)
   \( (7) \) x,x,z
   \( (m_{xy}) 0,0,0' \)

8. \( m' \)
   \( (8) \) x,x,z
   \( (m_{xy}) 0,0,0' \)

P4₂ c’m’ 4m’m’ Tetragonal
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 8 e 1        | (1) x,y,z [u,v,w]  
(2) x,y,z [u,v,w]  
(3) y,x,z+1/2 [v,u,w]  
(4) y,x,z+1/2 [v,u,w]  
(5) x,y,z+1/2 [u,v,w]  
(6) x,y,z+1/2 [u,v,w]  
(7) y,x,z [v,u,w]  
(8) y,x,z [v,u,w] |

| 4 d .m' | x,x,z [u,u,w]  
 x,x,z [u,u,w]  
 x,x,z+1/2 [u,u,w]  
 x,x,z+1/2 [u,u,w] |

| 4 c 2.. | 0,1/2,z [0,0,w]  
 1/2,0,z+1/2 [0,0,w]  
 0,1/2,z+1/2 [0,0,w]  
 1/2,0,z [0,0,w] |

| 2 b 2.m'm' | 1/2,1/2,z [0,0,w]  
 1/2,1/2,z+1/2 [0,0,w] |

| 2 a 2.m'm' | 0,0,z [0,0,w]  
 0,0,z+1/2 [0,0,w] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b b* = c/2</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2 b* = c</td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0
Origin on 2mm on 4\textsubscript{2} cm

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\)

Symmetry Operations

For \((0,0,0)\) + set

1. \((1')\) (0,0,0)
2. \((2)\) 0,0,z
   \(2_z\) 0,0,0
3. \((3)^*\) (0,0,1/2) 0,0,z
   \(4_z\) 0,0,1/2
4. \((4)^*\) (0,0,1/2) 0,0,z
   \(4_z^{-1}\) 0,0,1/2
5. \((5)\) c (0,0,1/2) x,0,z
   \(m_y\) 0,0,1/2
6. \((6)\) c (0,0,1/2) 0,y,z
   \(m_x\) 0,0,1/2
7. \((7)^*\) x,x,z
   \(m_y\) 0,0,0
8. \((8)^*\) x,x,z
   \(m_y\) 0,0,0

For \((1,0,0)'\) + set

1. \((1)^*\) (1,0,0)
   \(1',1,0,0)\)
2. \((2)'\) 1/2,0,z
   \(2_z\) 1,0,0\)
3. \((3)'\) (0,0,1/2) 1/2,1/2,z
   \(4_z\) 1,0,1/2\)
4. \((4)'\) (0,0,1/2) 1/2,-1/2,z
   \(4_z^{-1}\) 1,0,1/2\)
5. \((5)^*\) (1,0,1/2) x,0,z
   \(m_y\) 1,0,1/2\)
6. \((6)^*\) (0,0,1/2) 1/2,y,z
   \(m_x\) 1,0,1/2\)
7. \((7)^*\) (1/2,-1/2,0) x+1/2,y,z
   \(m_y\) 1,0,0\)
8. \((8)^*\) (1/2,1/2,0) x+1/2,y,z
   \(m_y\) 1,0,0\)
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 e</td>
<td>1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z+1/2 [v,u,w] (4) y,x,z+1/2 [v,u,w] (5) x,y,z+1/2 [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 d</td>
<td>..m</td>
<td>x,x,z [u,u,0] x,x,z [u,u,0] x,x,z+1/2 [u,u,0] x,x,z+1/2 [u,u,0]</td>
</tr>
<tr>
<td>8 c</td>
<td>2'</td>
<td>0,1/2,z [u,v,0] 0,1/2,z [u,v,0] 0,1/2,z+1/2 [u,v,0] 0,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td>4 b</td>
<td>2.mm</td>
<td>1/2,1/2,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a</td>
<td>2.mm</td>
<td>0,0,z [0,0,0] 0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{4mm} \) Along [1,0,0] \( p1m11' \) Along [1,1,0] \( p1m11' \)
\( a^* = a \quad b^* = b \quad a^* = b \quad b^* = c/2 \quad a^* = (-a + b)/2 \quad b^* = c \)
Origin at 0,0,z Origin at x,0,0 Origin at x,x,0
Origin on 2\textit{m}m' on 4\textit{m}1'

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\]

Symmetry Operations

For (0,0,0) + set

(1) \text{1} \quad (1)\begin{array}{l} \text{1} \\ \text{1}
\end{array} \begin{array}{l} \text{0,0,0} \\ \text{0,0,0}
\end{array}

(2) \text{2} \quad 0,0,z 
\begin{array}{l} \text{2} \\ \text{2}
\end{array} \begin{array}{l} 0,0,0 \\ 0,0,0
\end{array}

(3) 4\text{+}' \quad (0,0,1/2) \quad 0,0,z 
\begin{array}{l} 4\text{+}' \\ 4\text{+}'
\end{array} \begin{array}{l} (0,0,1/2) \\ (0,0,1/2)
\end{array}

(4) 4\text{-}' \quad (0,0,1/2) \quad 0,0,z 
\begin{array}{l} 4\text{-}' \\ 4\text{-}'
\end{array} \begin{array}{l} (0,0,1/2) \\ (0,0,1/2)
\end{array}

(5) c \quad (0,0,1/2) \quad x,0,z 
\begin{array}{l} c \\ c
\end{array} \begin{array}{l} (0,0,1/2) \\ (0,0,1/2)
\end{array}

(6) c' \quad (0,0,1/2) \quad 0,y,z 
\begin{array}{l} c' \\ c'
\end{array} \begin{array}{l} (0,0,1/2) \\ (0,0,1/2)
\end{array}

(7) m' \quad x,x,z 
\begin{array}{l} m' \\ m'
\end{array} \begin{array}{l} x,x,z \\ (m_{xy}|0,0,0)
\end{array}

(8) m' \quad x,x,z 
\begin{array}{l} m' \\ m'
\end{array} \begin{array}{l} x,x,z \\ (m_{xy}|0,0,0)
\end{array}

For (1,0,0)' + set

(1) \text{t}' \quad (1,0,0) 
\begin{array}{l} \text{t}' \\ \text{t}'
\end{array} \begin{array}{l} (1,0,0) \\ (1,0,0)
\end{array}

(2) \text{2}' \quad 1/2,0,z 
\begin{array}{l} \text{2}' \\ \text{2}'
\end{array} \begin{array}{l} 1/2,0,z \\ 1/2,0,z
\end{array}

(3) 4\text{+}' \quad (0,0,1/2) \quad 1/2,1/2,z 
\begin{array}{l} 4\text{+}' \\ 4\text{+}'
\end{array} \begin{array}{l} (0,0,1/2) \\ (0,0,1/2)
\end{array}

(4) 4\text{-}' \quad (0,0,1/2) \quad 1/2,-1/2,z 
\begin{array}{l} 4\text{-}' \\ 4\text{-}'
\end{array} \begin{array}{l} (0,0,1/2) \\ (0,0,1/2)
\end{array}

(5) n' \quad (1,0,1/2) \quad x,0,z 
\begin{array}{l} n' \\ n'
\end{array} \begin{array}{l} (1,0,1/2) \\ (1,0,1/2)
\end{array}

(6) c' \quad (0,0,1/2) \quad 1/2,y,z 
\begin{array}{l} c' \\ c'
\end{array} \begin{array}{l} (0,0,1/2) \\ (0,0,1/2)
\end{array}

(7) g \quad (1/2,-1/2,0) \quad x+1/2,x,z 
\begin{array}{l} g \\ g
\end{array} \begin{array}{l} (1/2,-1/2,0) \\ (1/2,-1/2,0)
\end{array}

(8) g \quad (1/2,1/2,0) \quad x+1/2,x,z 
\begin{array}{l} g \\ g
\end{array} \begin{array}{l} (1/2,1/2,0) \\ (1/2,1/2,0)
\end{array}
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 e 1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 (5)</td>
<td>x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>8 d ..m'</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>8 c 2'..</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td>4 b 2.m'm'</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 a 2.m'm'</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p\text{\textprime}1m1'</td>
</tr>
<tr>
<td>[0,0,1]</td>
<td>p\text{\textprime}1m1'</td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>p_2\text{\textprime}1m1</td>
</tr>
<tr>
<td>[0,0,2]</td>
<td>p\text{\textprime}1m1'</td>
</tr>
<tr>
<td>[0,0,0]</td>
<td>p\text{\textprime}1m1'</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,0,0
Origin on 2mm on 21m

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \)

Symmetry Operations

1. \((1)\ 1\ (0,0,0)\)
2. \((2)\ 0,0,z\ (0,0,0)\)
3. \((3)\ 0,0,1/2\ (0,1/2,1/2)\)
4. \((4)\ 0,1/2,1/2\ (1/2,0,z)\)
5. \((5)\ n\ (1/2,0,1/2)\ (x,1/4,z)\)
6. \((6)\ n\ (0,1/2,1/2)\ (1/4,y,z)\)
7. \((7)\ m\ x,x,z\ (m_{x}x,0,0)\)
8. \((8)\ m\ x,x,z\ (m_{y}y,0,0)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>8</th>
<th>d</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>..m</td>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x+1/2,x+1/2,z+1/2 [u,u,0]</td>
<td>x+1/2,x+1/2,z+1/2 [u,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>2.mm</td>
<td>0,0,z [0,0,0]</td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm

\( a^* = a \quad b^* = b \)

Origin at 0,1/2,z

Along [1,0,0] c\(_{\text{p}}\)1m1

\( a^* = b \quad b^* = c \)

Origin at x,0,0

Along [1,1,0] p1m11'

\( a^* = (-a + b)/2 \quad b^* = c \)

Origin at x,x,0

Origin at x,0,0
**Origin** on 2mm1' on 21m1'

**Asymmetric unit**

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1; \quad x \leq y\]

**Symmetry Operations**

**For 1 + set**

1. \((1)\) 1
2. \((2)\) 2 0,0,z
   \( (2z) \) 0,0,0
3. \((3)\) 4* (0,0,1/2) 0,1/2,z
   \( (4z) \) 1/2,1/2,1/2
4. \((4)\) 4' (0,0,1/2) 1/2,0,z
   \( (4z) \) 1/2,1/2,1/2
5. \((5)\) n (1/2,0,1/2) \(x,1/4,z\)
6. \((6)\) n (0,1/2,1/2) 1/4,y,z
   \( (m_x) \) 1/2,1/2,1/2
7. \((7)\) m \(x,x,z\)
   \( (m_{xy}) \) 0,0,0
8. \((8)\) m \(x,x,z\)
   \( (m_{xy}) \) 0,0,0

**For 1' + set**

1. \((1')\) 1'
2. \((2')\) 2' 0,0,z
   \( (2z) \) 0,0,0
3. \((3')\) 4* (0,0,1/2) 0,1/2,z
   \( (4z) \) 1/2,1/2,1/2
4. \((4')\) 4' (0,0,1/2) 1/2,0,z
   \( (4z) \) 1/2,1/2,1/2
5. \((5')\) n' (1/2,0,1/2) \(x,1/4,z\)
6. \((6')\) n' (0,1/2,1/2) 1/4,y,z
   \( (m_x) \) 1/2,1/2,1/2
7. \((7')\) m' \(x,x,z\)
   \( (m_{xy}) \) 0,0,0
8. \((8')\) m' \(x,x,z\)
   \( (m_{xy}) \) 0,0,0
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8  d  11'</td>
<td>x,y,z [0,0,0]</td>
<td>(1)</td>
</tr>
<tr>
<td></td>
<td>x,y,z [0,0,0]</td>
<td>(2)</td>
</tr>
<tr>
<td></td>
<td>x,y,z [0,0,0]</td>
<td>(3)</td>
</tr>
<tr>
<td></td>
<td>y+1/2,x+1/2,z+1/2 [0,0,0]</td>
<td>(4)</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td>(5)</td>
</tr>
<tr>
<td></td>
<td>y,x,z [0,0,0]</td>
<td>(6)</td>
</tr>
<tr>
<td></td>
<td>x,x,z [0,0,0]</td>
<td>(7)</td>
</tr>
<tr>
<td></td>
<td>y,x,z [0,0,0]</td>
<td>(8)</td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4gm1'</th>
<th>Along [1,0,0]</th>
<th>c1m1'</th>
<th>Along [1,1,0]</th>
<th>p1m11'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -(a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,1/2,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on 2mm on 21m

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\]

**Symmetry Operations**

1. \(1\)
   - \((0,0,0)\)
2. \(2\)
   - \(0,0,z\)
   - \((2z,0,0)\)
3. \(4^+\) \((0,0,1/2)\)
   - \((0,1/2,1/2)\)
   - \((1/2,1/2,1/2)\)
4. \(4^-\) \((0,0,1/2)\)
   - \((1/2,0,1/2)\)
   - \((1/2,1/2,1/2)\)
5. \(n'\) \((1/2,0,1/2)\)
   - \(x,1/4,z\)
   - \((m_y,1/2,1/2,1/2)\)
6. \(n'\) \((0,1/2,1/2)\)
   - \(1/4,y,z\)
   - \((m_x,1/2,1/2,1/2)\)
7. \(m\)
   - \(x,x,z\)
   - \((m_{xy},0,0)\)
8. \(m\)
   - \(x,x,z\)
   - \((m_{xy},0,0)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

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<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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</tr>
</tbody>
</table>

| 8 | d | 1 | (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] |
|   |   |   | (3) y+1/2,x+1/2,z+1/2 [v,u,w] | (4) y+1/2,x+1/2,z+1/2 [v,u,w] |
|   |   |   | (5) x+1/2,y+1/2,z+1/2 [u,v,w] | (6) x+1/2,y+1/2,z+1/2 [u,v,w] |
|   |   |   | (7) y,x,z [v,u,w] | (8) y,x,z [v,u,w] |

| 4 | c | m | x,x,z [u,u,0] | x,x,z [u,u,0] |
|   |   |   | x+1/2,x+1/2,z+1/2 [u,u,0] | x+1/2,x+1/2,z+1/2 [u,u,0] |

| 4 | b | 2.. | 0,1/2,z [0,0,w] | 0,1/2,z+1/2 [0,0,w] |
|   |   |   | 1/2,0,z+1/2 [0,0,w] | 1/2,0,z+1/2 [0,0,w] |

| 2 | a | 2.mm | 0,0,z [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4'g'm

a* = a  b* = b
Origin at 0,1/2,z

Along [1,0,0] c1m'1

a* = b  b* = c
Origin at x,0,0

Along [1,1,0] p1m11'

a* = (a + b)/2  b* = c
Origin at x,x,0
Origin on 2$m'$m' on 21$m'\text{'}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x < y$

Symmetry Operations

1. $1$
   
   (1) $0,0,0$

2. $2$ $0,0,z$
   
   (2) $2z,0,0,0$

3. $4'$ $(0,0,1/2) 0,1/2,z$
   
   (3) $4z,1/2,1/2,1/2'$

4. $4'$ $(0,0,1/2) 1/2,0,z$
   
   (4) $4z^{-1},1/2,1/2,1/2'$

5. $n (1/2,0,1/2) x,1/4,z$
   
   (5) $m_y (1/2,1/2,1/2)$

6. $n (0,1/2,1/2) 1/4,y,z$
   
   (6) $m_x (1/2,1/2,1/2)$

7. $m' x,x,z$
   
   (7) $m_{xy} (0,0,0)'$

8. $m' x,x,z$
   
   (8) $m_{xy} (0,0,0)'$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>d 1 (1) x,y,z [u,v,w]</td>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u.w]</td>
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<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
</tbody>
</table>

| 4            | c ..m’ x,x,z [u,u,w]             |
|              | x,x,z [u,u,w]                    |
|              | +1/2,x+1/2,z+1/2 [u,u,w]         |
|              | +1/2,x+1/2,z+1/2 [u,u,w]         |
|              | 0,1/2,z+1/2 [0,0,w]              |
|              | 1/2,0,z+1/2 [0,0,w]              |
|              | 1/2,0,z [0,0,w]                  |

Symmetry of Special Projections

Along [0,0,1] p4'gm'  
Along [1,0,0] c_p'1m'1  
Along [1,1,0] p1m'1

\( a^* = a \quad b^* = b \quad a^* = b \quad b^* = c \quad a^* = (-a + b)/2 \quad b^* = c \)

Origin at 0,1/2,z  
Origin at x,0,0  
Origin at x,x,0
Origin on 2m'm' on 21m'

Asymmetric unit: 

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \]

Symmetry Operations:

1. 1
2. \(2 \cdot 0,0,z\) (2
3. \(4^+ (0,0,1/2) 0,1/2,z\)
4. \(4^- (0,0,1/2) 1/2,0,z\)
5. \(n' (1/2,0,1/2) x,1/4,z\)
6. \(n' (0,1/2,1/2) 1/4,y,z\)
7. \(m' x,x,z\)
8. \(m' x,x,z\)

\(m_y,1/2,1/2,1/2\)'

\(m_{xy},0,0,0\)'

102.5.856 - 1 - 1705
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 d 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,y+1/2,z+1/2 [v,u,w]</td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(4) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
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<td>y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(5) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(6) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
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<td>y,x,z [v,u,w]</td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
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<td>y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 c m'</td>
<td>x,z [u,u,w]</td>
<td>x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,z [u,u,w]</td>
<td>x,z [u,u,w]</td>
</tr>
<tr>
<td>4 b 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a m' m'</td>
<td>0,0,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p4g'm'
  - a* = a
  - b* = b

- Along [1,0,0] c1m'1
  - a* = b
  - b* = c

- Along [1,1,0] p1m'1
  - a* = (-a + b)/2
  - b* = c

Origin at 0,1/2,z
Origin at x,0,0
Origin at x,x,0
P4, nm
102.6.857
PI,4, nm

4mm1'
Tetragonal
Origin on 2mm on 21m

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 4^* (0,0,1/2) \quad 0,1/2,z \\
(4) & \quad 4^* (0,0,1/2) \quad 1/2,0,z \\
(5) & \quad n \ (1/2,0,1/2) \quad x,1/2,z \\
(6) & \quad n \ (0,1/2,1/2) \quad 1/2,y,z \\
(7) & \quad m \ x,x,z \\
(8) & \quad m \ x,x,z \\
\end{align*}
\]

\[
\begin{align*}
(1)_* & \quad 0,0,0 \\
(2)_* & \quad 0,0,0 \\
(3)_* & \quad 0,0,0 \\
(4)_* & \quad 0,0,0 \\
(5)_* & \quad 1/2,1/2,1/2 \\
(6)_* & \quad 1/2,1/2,1/2 \\
(7)_* & \quad 0,0,0 \\
(8)_* & \quad 0,0,0 \\
\end{align*}
\]

For \((1,0,0)' + \) set

\[
\begin{align*}
(1) & \quad t' \ (1,0,0) \\
(2) & \quad 2' \quad 1/2,0,z \\
(3) & \quad 4^* (0,0,1/2) \quad -1/2,0,z \\
(4) & \quad 4^* (0,0,1/2) \quad 0,1/2,z \\
(5) & \quad n' \ (3/2,0,1/2) \quad x,1/4,z \\
(6) & \quad n' \ (0,1/2,1/2) \quad 3/4,y,z \\
(7) & \quad g' \ (1/2,-1/2,0) \quad x+1/2,x,z \\
(8) & \quad g' \ (1/2,1/2,0) \quad x+1/2,x,z \\
\end{align*}
\]

\[
\begin{align*}
(1)_* & \quad 1,0,0 \\
(2)_* & \quad 1,0,0 \\
(3)_* & \quad 3/2,1/2,1/2 \\
(4)_* & \quad 3/2,1/2,1/2 \\
(5)_* & \quad 3/2,1/2,1/2 \\
(6)_* & \quad 3/2,1/2,1/2 \\
(7)_* & \quad 0,0,0 \\
(8)_* & \quad 0,0,0 \\
\end{align*}
\]

Generators selected \((1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).\)

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>((0,0,0) + (1,0,0)' +)</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>(c) ..m (x,x,z [u,u,0]) (x,x,z [u,u,0]) (x+1/2,x+1/2,z+1/2 [u,u,0] x+1/2,x+1/2,z+1/2 [u,u,0] )</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>(b) 2'.. (0,1/2,z [u,v,0]) (1/2,0,z+1/2 [u,v,0] 1/2,0,z+1/2 [u,v,0] 1/2,0,z [v,u,0])</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>(a) 2.mm (0,0,z [0,0,0]) (1/2,1/2,z+1/2 [0,0,0])</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \(p4gm1'\)  
Along \([1,0,0]\) \(c1m11'\)  
Along \([1,1,0]\) \(p1m11'\)  
\(a^* = a \) \(b^* = b\)  
\(a^* = b \) \(b^* = c\)  
\(a^* = (a + b)/2 \) \(b^* = c\)  
Origin at \(0,1/2,z\)  
Origin at \(x,0,0\)  
Origin at \(x,x,0\)
Origin on 2m’ on 21m’

Asymmetric unit  

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\]

Symmetry Operations

For \((0,0,0) +\) set

\[(1) 1 \quad (2) 2 \quad (3) 4^* (0,0,1/2) \quad (4) 4^* (0,0,1/2) \quad (5) n' (1/2,0,1/2) \quad (6) n' (0,1/2,1/2) \quad (7) m' x,x,z \quad (8) m' x,x,z\]

For \((1,0,0)' +\) set

\[(1) t' (1,0,0) \quad (2) 2' \quad (3) 4^* (0,0,1/2) \quad (4) 4^* (0,0,1/2) \quad (5) n (3/2,0,1/2) \quad (6) n (0,1/2,1/2) \quad (7) g (1/2,-1/2,0) \quad (8) g (1/2,1/2,0)\]

Generators selected  

\((1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).\)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{array}{cccc}
\text{Multiplicity} & \text{Wyckoff letter} & \text{Site Symmetry} & \text{Coordinates} \\
16 & d & 1 & (0,0,0) + \\
8 & c & ..m' & (1,0,0)' + \\
8 & b & 2'.. & 0,1/2,z [u,v,0] \\
4 & a & 2.m'm' & 0,0,z [0,0,w] \\
\end{array}
\]

Symmetry of Special Projections

Along \([0,0,1]\)  
\(p4gm1'\)  
Along \([1,0,0]\)  
\(c1m11'\)  
Along \([1,1,0]\)  
\(p_{1}c1m1\)

\(a^* = a \quad b^* = b\)

Origin at \(0,1/2,z\)

\(a^* = b \quad b^* = c\)

Origin at \(x,0,0\)

\(a^* = (-a + b)/2 \quad b^* = c\)

Origin at \(x,x,1/2\)
Origin on 4cc

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. \( 1 \)
   \( (1,0,0,0) \)

2. 2 0,0,z
   \( (2_1,0,0,0) \)

3. 4 0,0,z
   \( (4_z,0,0,0) \)

4. 4 0,0,z
   \( (4_{-1},0,0,0) \)

5. c (0,0,1/2) x,0,z
   \( (m_y,0,0,1/2) \)

6. c (0,0,1/2) 0,y,z
   \( (m_x,0,0,1/2) \)

7. c (0,0,1/2) x,\bar{x},z
   \( (m_{xy},0,0,1/2) \)

8. c (0,0,1/2) x,x,z
   \( (m_{xy},0,0,1/2) \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 c 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 4..</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm

\( a^* = a \) \hspace{1cm} \( b^* = b \)

Origin at 0,0,z

Along [1,0,0] \( p_{2b\cdot1m'1} \)

\( a^* = b \) \hspace{1cm} \( b^* = c/2 \)

Origin at x,0,0

Along [1,1,0] \( p_{2b\cdot1m'1} \)

\( a^* = (-a + b)/2 \) \hspace{1cm} \( b^* = c/2 \)

Origin at x,x,0
Origin on 4cc1'

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

For 1 + set

\begin{align*}
(1) & \quad 1 \quad (1 | 0,0,0) \\
(2) & \quad 2 \quad 0,0,z \quad (2_z | 0,0,0) \\
(3) & \quad 4' \quad 0,0,z \quad (4_z | 0,0,0) \\
(4) & \quad 4' \quad 0,0,z \quad (4_z^{-1} | 0,0,0) \\
(5) & \quad c (0,0,1/2) \quad x,0,z \quad (m_y | 0,0,1/2) \\
(6) & \quad c (0,0,1/2) \quad 0,y,z \quad (m_x | 0,0,1/2) \\
(7) & \quad c (0,0,1/2) \quad x,x,z \quad (m_{xy} | 0,0,1/2) \\
(8) & \quad c (0,0,1/2) \quad x,x,z \quad (m_{xy} | 0,0,1/2) \\
\end{align*}

For 1' + set

\begin{align*}
(1) & \quad 1' \quad (1 | 0,0,0) \\
(2) & \quad 2' \quad 0,0,z \quad (2_z | 0,0,0)' \\
(3) & \quad 4' \quad 0,0,z \quad (4_z | 0,0,0)' \\
(4) & \quad 4' \quad 0,0,z \quad (4_z^{-1} | 0,0,0)' \\
(5) & \quad c' (0,0,1/2) \quad x,0,z \quad (m_y | 0,0,1/2)' \\
(6) & \quad c' (0,0,1/2) \quad 0,y,z \quad (m_x | 0,0,1/2)' \\
(7) & \quad c' (0,0,1/2) \quad x,x,z \quad (m_{xy} | 0,0,1/2)' \\
(8) & \quad c' (0,0,1/2) \quad x,x,z \quad (m_{xy} | 0,0,1/2)' \\
\end{align*}
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<tbody>
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<td>1' +</td>
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<tr>
<td>8</td>
<td>d</td>
<td>11'</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4..1'</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>2..1'</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4..1'</td>
</tr>
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</table>

<table>
<thead>
<tr>
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<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>1 +</td>
<td>1' +</td>
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<tr>
<td>(1) x,y,z</td>
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</tr>
<tr>
<td>(2) x,y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(3) y,x,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(4) y,x,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(6) x,y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(7) y,x,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(8) y,x,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(9) 0,1/2 ,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(10) 0,1/2 ,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(11) 0,1/2 ,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(12) 0,1/2 ,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(13) 0,1/2 ,z</td>
<td>[0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [1,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>p4mm1'</td>
<td>p1m11'</td>
<td>p1m11'</td>
</tr>
<tr>
<td>b* = b</td>
<td>a* = b</td>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 4'c'c

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$
(1) $0,0,0$

(2) $2 \ 0,0,z$
(2) $z, 0,0,0$

(3) $4^{+} \quad 0,0,z$
(4) $z, 0,0,0'$

(4) $4^{-} \quad 0,0,z$
(4) $z^{-1}, 0,0,0$

(5) $c' \ (0,0,1/2) \ x,0,z$
(5) $m_y, 0,0,1/2$

(6) $c' \ (0,0,1/2) \ 0,y,z$
(6) $m_x, 0,0,1/2$

(7) $c \ (0,0,1/2) \ x,x,z$
(7) $m_{xy}, 0,0,1/2$

(8) $c \ (0,0,1/2) \ x,x,z$
(8) $m_{x+y}, 0,0,1/2$
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<tr>
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<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>c 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 4'..</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'm'm

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

Along [1,0,0] p1m'1

\[ a^* = b \quad b^* = c/2 \]

Origin at x,0,0

Along [1,1,0] p_{21}.1m'1

\[ a^* = (-a + b)/2 \quad b^* = c/2 \]

Origin at x,x,0
Origin on 4'cc'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) 0,0,0

(3) 4* 0,0,z
(4) 0,0,0

(4) 4* 0,0,0'
(4) 0,0,0'

(5) c (0,0,1/2) x,0,z
(m_x|0,0,1/2)

(6) c (0,0,1/2) 0,y,z
(m_y|0,0,1/2)

(7) c' (0,0,1/2) x,x,z
(m_x|0,0,1/2)

(8) c' (0,0,1/2) x,x,z
(m_y|0,0,1/2)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>8</td>
<td>d 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(5) x,y,z+1/2 [u,v,w]</td>
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<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
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<tr>
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<td>1/2,0,z [0,0,w]</td>
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<td>0,1/2,z+1/2 [0,0,w]</td>
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<td>2</td>
<td>b 4</td>
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</tr>
<tr>
<td>2</td>
<td>a 4</td>
<td>0,0,z [0,0,0]</td>
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<tr>
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<td></td>
<td>0,0,z+1/2 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4'mmm'  Along [1,0,0] p2b*1m'1  Along [1,1,0] p1m'1
a* = a  b* = b  a* = b  b* = c/2  a* = (-a + b)/2  b* = c/2
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
Origin on 4c'c'

Asymmetric unit  
0 ≤ x ≤ 1/2;  
0 ≤ y ≤ 1/2;  
0 ≤ z ≤ 1/2

Symmetry Operations

(1) 1  
(1) [0,0,0]

(2) 2 0,0,z  
(2z) 0,0,0

(3) 4' 0,0,z  
(4z) 0,0,0

(4) 4' 0,0,z  
(4z') 0,0,0

(5) c' (0,0,1/2) x,0,z  
(my) [0,0,1/2]'

(6) c' (0,0,1/2) 0,y,z  
(mx) [0,0,1/2]'

(7) c' (0,0,1/2) x,0,z  
(mz) [0,0,1/2]'

(8) c' (0,0,1/2) x,x,z  
(mxy) [0,0,1/2]'
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Coordinates</th>
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<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
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<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>0,0,z [0,0,w]</td>
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**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Along [0,0,1]</th>
<th>p4m' ( \cdot ) m'</th>
<th>Along [1,0,0]</th>
<th>p1m' ( \cdot ) 1</th>
<th>Along [1,1,0]</th>
<th>p1m' ( \cdot ) 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{a}^* = \mathbf{a} ) ( \mathbf{b}^* = \mathbf{b} )</td>
<td>( \mathbf{a}^* = \mathbf{b} ) ( \mathbf{b}^* = \mathbf{c}/2 )</td>
<td>( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 ) ( \mathbf{b}^* = \mathbf{c}/2 )</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
**Symmetry Operations**

For \((0,0,0)\) + set

1. \((1,0,0)\)
2. \((2,0,0,z)\)
3. \((4^+, 0,0,z)\)
4. \((4^-, 0,0,z)\)

5. \((c, 0,0,1/2, x,0,z)\)
6. \((c, 0,0,1/2, 0,y,z)\)
7. \((c, 0,0,1/2, x,\bar{x},z)\)
8. \((c, 0,0,1/2, x,x,z)\)

For \((1,0,0)\)' + set

1. \((t', 1,0,0)\)
2. \((2', 1/2,0,z)\)
3. \((4'^+, 1/2,1/2,z)\)
4. \((4'^-, 1/2,-1/2,z)\)

5. \((n', 1,0,1/2, x,0,z)\)
6. \((c', 0,0,1/2, 1/2,y,z)\)
7. \((n', 1/2,-1/2,1/2, x+1/2,\bar{x},z)\)
8. \((n', 1/2,1/2,1/2, x+1/2,x,z)\)
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>(1) x,y,z [u,v,w]</td>
<td>(1,0,0)' +</td>
</tr>
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<td>(2) x,y,z [u,v,w]</td>
<td></td>
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<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
<td></td>
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<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
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<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
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</tr>
<tr>
<td></td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>c</td>
<td>0,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(2')</td>
<td>1/2,0,z [v,u,0]</td>
</tr>
<tr>
<td></td>
<td>(3)</td>
<td>0,1/2,z+1/2 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(4)</td>
<td>1/2,0,z+1/2 [v,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4')</td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(4)</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p\_4mm \)

Along [1,0,0] \( p1m1 \)

Along [1,1,0] \( p\_1m1 \)

\( a^* = a \quad b^* = b \)

\( a^* = b \quad b^* = c/2 \)

\( a^* = (-a + b)/2 \quad b^* = c/2 \)

Origin at 0,0,z

Origin at x,0,0

Origin at x-1/4,x+1/4,0
Origin on 4'cc'

Asymmetric unit \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0)\) + set

(1) \(1\)
   \((1\mid0,0,0)\)

(2) \(2\ 0,0,z\)
   \((2\z|0,0,0)\)

(3) \(4^*\ 0,0,z\)
   \((4\z|0,0,0)\)'

(4) \(4^*\ 0,0,z\)
   \((4\z^{-1}|0,0,0)\)'

(5) \(c\ (0,0,1/2)\) \(x,0,z\)
   \((m_y|0,0,1/2)\)

(6) \(c\ (0,0,1/2)\) \(0,y,z\)
   \((m_x|0,0,1/2)\)

(7) \(c'\ (0,0,1/2)\) \(x,x,z\)
   \((m_{xy}|0,0,1/2)\)'

(8) \(c'\ (0,0,1/2)\) \(x,x,z\)
   \((m_{xy}^{-1}|0,0,1/2)\)'

For \((1,0,0')\) + set

(1) \(t'\) \((1,0,0)\)
   \((1\mid1,0,0')\)

(2) \(2'\ 1/2,0,z\)
   \((2\z|1,0,0')\)

(3) \(4^*\ 1/2,1/2,z\)
   \((4\z|1,0,0)\)

(4) \(4^*\ 1/2,-1/2,z\)
   \((4\z^{-1}|1,0,0)\)

(5) \(n'\ (1,0,1/2)\) \(x,0,z\)
   \((m_y|1,0,1/2)\)

(6) \(c'\ (0,0,1/2)\) \(1/2,y,z\)
   \((m_x|1,0,1/2)\)'

(7) \(n\ (1/2,-1/2,1/2)\) \(x+1/2,x,z\)
   \((m_{xy}|1,0,1/2)\)

(8) \(n\ (1/2,1/2,1/2)\) \(x+1/2,x,z\)
   \((m_{xy}^{-1}|1,0,1/2)\)
### Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Symmetry of Special Projections</th>
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<td>16 d 1</td>
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<td>p_4m'm'</td>
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<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>a^* = a  b^* = b</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td>a^* = b  b^* = c/2</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
<td>a^* = (-a + b)/2  b^* = c/2</td>
</tr>
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<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>Origin at 1/2,1/2,z</td>
</tr>
<tr>
<td>8 c 2'..</td>
<td>(1,0,0)' +</td>
<td>p_1m'1'</td>
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<tr>
<td>0,1/2,z [u,v,0]</td>
<td>1/2,0,z [v,u,0]</td>
<td>a^* = a  b^* = b</td>
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<td>4 b 4..</td>
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<td>p_2x.1m1</td>
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<tr>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
<td>a^* = (-a + b)/2  b^* = c/2</td>
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<tr>
<td>4 a 4'..</td>
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<td></td>
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<tr>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
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</tbody>
</table>
Origin on 41n

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

(1) 1
(1') 0,0,0

(2) 2 \(0,0,z\)
(2') \(0,0,0\)

(3) 4' \(0,0,z\)
(4') \(0,0,0\)

(5) \(n\) \((1/2,0,1/2)\) \(x,1/4,z\)

(6) \(n\) \((0,1/2,1/2)\) \(1/4,y,z\)

(7) \(c\) \((0,0,1/2)\) \(x+1/2,\bar{x},z\)

(8) \(n\) \((1/2,1/2,1/2)\) \(x,x,z\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tbody>
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<td>(3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w] (6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
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<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w] (8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<tr>
<td>4 b 2..</td>
<td>0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4gm
\[
a^* = a \quad b^* = b
\]
Origin at 0,0,z

Along [1,0,0] c\(_p\)1m'1
\[
a^* = b \quad b^* = c
\]
Origin at x,0,0

Along [1,1,0] p\(_{21}\)1m'1
\[
a^* = (-a + b)/2 \quad b^* = c/2
\]
Origin at x,x,0
Origin on 41n1’

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\]

Symmetry Operations

For 1 + set

1. \(1\)
2. \(2\) 0,0,z
3. \(4^+\) 0,0,z
4. \(4^-\) 0,0,z
5. \(n\) (1/2,0,1/2) z,1/4,z
6. \(n’\) (0,1/2,1/2) 1/4,y,z
7. \(c\) (0,0,1/2) x+1/2,x,z
8. \(n\) (1/2,1/2,1/2) x,x,z

For 1’ + set

1. \(1’\)
2. \(2’\) 0,0,z
3. \(4^{+’}\) 0,0,z
4. \(4^{-’}\) 0,0,z
5. \(n’\) (1/2,0,1/2) z,1/4,z
6. \(n’\) (0,1/2,1/2) 1/4,y,z
7. \(c’\) (0,0,1/2) x+1/2,x,z
8. \(n’\) (1/2,1/2,1/2) x,x,z
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

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<td>1' +</td>
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<td>8 c 11'</td>
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<tr>
<td></td>
<td>(2) x̅,y̅,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y̅,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) y̅,x̅,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2, y+1/2, z+1/2 [0,0,0]</td>
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<td>(6) x̅+1/2, y̅+1/2, z+1/2 [0,0,0]</td>
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<td>(7) y̅+1/2, x̅+1/2, z+1/2 [0,0,0]</td>
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<td>(8) y+1/2, x+1/2, z+1/2 [0,0,0]</td>
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<tr>
<td>4 b 2..1'</td>
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<td>1/2,0,z [0,0,0]</td>
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Symmetry of Special Projections

<table>
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<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>p4gm1'</th>
<th>Along [1,0,0]</th>
<th>c1m1'</th>
<th>Along [1,1,0]</th>
<th>p1m1'</th>
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<tbody>
<tr>
<td>a* = a</td>
<td></td>
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<td>a* = b</td>
<td>c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
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<td>b* = b</td>
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<td></td>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
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</tbody>
</table>
Origin on 4'1n

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

**Symmetry Operations**

1. (1) 1
   (1' | 0,0,0)
2. (2) 2 0,0,z
   (2z | 0,0,0)
3. (3) 4+ · 0,0,z
   (4z | 0,0,0)'
4. (4) 4+ · 0,0,z
   (4z⁻¹ | 0,0,0)'
5. (5) n' (1/2,0,1/2)
   x,1/4,z
   (m|y,1/2,1/2,1/2)'
6. (6) n' (0,1/2,1/2)
   1/4,y,z
   (m|x,1/2,1/2,1/2)'
7. (7) c (0,0,1/2)
   x+1/2,x,z
   (m|y,1/2,1/2,1/2)
8. (8) n (1/2,1/2,1/2)
   x,x,z
   (m|y,1/2,1/2,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>(1) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p4'g'm</td>
</tr>
<tr>
<td>a* = a  b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
</tr>
</tbody>
</table>
Origin on 4'1n'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

1. 1
   (1) [0,0,0]

2. 2 0,0,z
   (2) [0,0,0]

3. 4 0,0,z
   (3) [0,0,0]

4. 4 0,0,z
   (4) [0,0,0]

5. n (1/2,0,1/2) x,1/4,z
   (5) (1/2,0,1/2) x,1/4,z

6. n (0,1/2,1/2) 1/4,y,z
   (6) (0,1/2,1/2) 1/4,y,z

7. c' (0,0,1/2) x+1/2, x,z
   (7) (0,0,1/2) x+1/2, x,z

8. n' (1/2,1/2,1/2) x,x,z
   (8) (1/2,1/2,1/2) x,x,z

104.4.869 - 1 - 1731
**Generators selected**

1; t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
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<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 b 2</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 4''</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'gm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a   b* = b</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c_p,1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b   b* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2   b* = c/2</td>
<td></td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin on 41n'**

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

1. \[ 1 \]
   \[ (1|0,0,0) \]

2. \[ 2 \]
   \[ (2z|0,0,0) \]

3. \[ 4^+ \]
   \[ (4z|0,0,0) \]

4. \[ 4^- \]
   \[ (4z^{-1}|0,0,0) \]

5. \[ n' \]
   \[ (1/2,0,1/2) \]
   \[ x,1/4,z \]
   \[ (m_y|1/2,1/2,1/2)' \]

6. \[ n' \]
   \[ (0,1/2,1/2) \]
   \[ 1/4,y,z \]
   \[ (m_x|1/2,1/2,1/2)' \]

7. \[ c' \]
   \[ (0,0,1/2) \]
   \[ x+1/2,x,z \]
   \[ (m_{xy}|1/2,1/2,1/2)' \]

8. \[ n' \]
   \[ (1/2,1/2,1/2) \]
   \[ x,x,z \]
   \[ (m_{xy}|1/2,1/2,1/2)' \]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>c 1</td>
</tr>
<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3)</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(5)</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(7)</td>
<td>y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

| 4            | b 2..       |
| 0,1/2,z [0,0,w] | 1/2,0,z [0,0,w] | 1/2,0,z+1/2 [0,0,w] | 0,1/2,z+1/2 [0,0,w] |

| 2            | a 4..       |
| 0,0,z [0,0,w] | 1/2,1/2,z+1/2 [0,0,w] |

Symmetry of Special Projections

Along [0,0,1] p4g'm' Along [1,0,0] c1m'1 Along [1,1,0] p1m'1
a* = a   b* = b   a* = b   b* = c   a* = (-a + b)/2   b* = c/2
Origin at 0,0,z   Origin at x,0,0   Origin at x,x,0
**Origin** on 2mm on $4_2mc$

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

1. \[ 1 \]
   \[ 1 | 0,0,0 \]

2. \[ 2 \]
   \[ 0,0,z \]
   \[ (2_z | 0,0,0) \]

3. \[ 4^+ \]
   \[ (0,0,1/2) \]
   \[ 0,0,z \]
   \[ (4_z | 0,0,1/2) \]

4. \[ 4^- \]
   \[ (0,0,1/2) \]
   \[ 0,0,z \]
   \[ (4_z^{-1} | 0,0,1/2) \]

5. \[ m \]
   \[ x,0,z \]
   \[ (m_y | 0,0,0) \]

6. \[ m \]
   \[ 0,y,z \]
   \[ (m_x | 0,0,0) \]

7. \[ c \]
   \[ (0,0,1/2) \]
   \[ x,x,z \]
   \[ (m_{xy} | 0,0,1/2) \]

8. \[ c \]
   \[ (0,0,1/2) \]
   \[ x,x,z \]
   \[ (m_{xy}^{-1} | 0,0,1/2) \]
Continued

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y,x,z+1/2 [v,u,w]</td>
<td>(4) y,x,z+1/2 [v,u,w]</td>
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<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 e</td>
<td>x,1/2,z [0,v,0]</td>
<td>x,1/2,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,x,z+1/2 [v,0,0]</td>
<td>1/2,x,z+1/2 [v,0,0]</td>
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<tr>
<td>4 d</td>
<td>x,0,z [0,v,0]</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
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<td>0,x,z+1/2 [v,0,0]</td>
<td>0,x,z+1/2 [v,0,0]</td>
</tr>
<tr>
<td>2 c</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
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<tr>
<td>2 a</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm

Along [1,0,0] p1m11'

Along [1,1,0] p21m1

**Origin at 0,0,z**

**a** = a  **b** = b

**Origin at x,0,0**

**a** = b  **b** = c
**Origin** on 2mm1' on $4_2\text{mc1}'$

**Asymmetric unit** \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

**Symmetry Operations**

For 1 + set

1. \(1\)
   1' \(0,0,0\)
   \(0,0,0\)'

2. \(2\)
   2' \(0,0,0\)
   \(0,0,0\)'

3. \(4^+ (0,0,1/2)\)
   \(4^+ (0,0,1/2)\)
   \(4z\|0,0,1/2\)
   \(4z^{-1} \|0,0,1/2\)

4. \(4^- (0,0,1/2)\)
   \(4^- (0,0,1/2)\)
   \(4z\|0,0,1/2\)
   \(4z^{-1} \|0,0,1/2\)

For 1' + set

5. \(m\) \(x,0,z\)
   \(m' \|0,0,0\)
   \(m' \|0,0,0\)'

6. \(m\) \(y,0,z\)
   \(m' \|0,0,0\)
   \(m' \|0,0,0\)'

7. \(c (0,0,1/2)\)
   \(c (0,0,1/2)\)
   \(m_{xy} \|0,0,1/2\)
   \(m_{xy} \|0,0,1/2\)'

8. \(c (0,0,1/2)\)
   \(c (0,0,1/2)\)
   \(m_{xy} \|0,0,1/2\)
   \(m_{xy} \|0,0,1/2\)'

---

105.2.872 - 1 - 1737
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
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</thead>
<tbody>
<tr>
<td>1 +</td>
<td>1' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>f 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z+1/2 [0,0,0]</td>
<td>(3) y,x,z+1/2 [0,0,0]</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+1/2 [0,0,0]</td>
<td>(4) y,x,z+1/2 [0,0,0]</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>e .m.1'</td>
<td>x,1/2,z [0,0,0]</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>x,1/2,z [0,0,0]</td>
<td>x,1/2,z [0,0,0]</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>1/2,x,z+1/2 [0,0,0]</td>
<td>1/2,x,z+1/2 [0,0,0]</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>1/2,x,z+1/2 [0,0,0]</td>
<td>1/2,x,z+1/2 [0,0,0]</td>
<td>4</td>
</tr>
<tr>
<td>2</td>
<td>c 2mm.1'</td>
<td>0,1/2,z [0,0,0]</td>
<td>2</td>
</tr>
<tr>
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<td>1/2,0,z+1/2 [0,0,0]</td>
<td>1/2,0,z+1/2 [0,0,0]</td>
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</tr>
<tr>
<td>2</td>
<td>b 2mm.1'</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>2</td>
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<tr>
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<td>1/2,1/2,z+1/2 [0,0,0]</td>
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</tr>
<tr>
<td>2</td>
<td>a 2mm.1'</td>
<td>0,0,z [0,0,0]</td>
<td>2</td>
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<tr>
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<td>0,0,z+1/2 [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
<td>2</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm1'      Along [1,0,0] p1m11'      Along [1,1,0] p1m11'
a* = a   b* = b     a* = b   b* = c       a* = -(a + b)/2   b* = c/2
Origin at 0,0,z    Origin at x,0,0    Origin at x,x,0
Origin on 2m’m’ on 4_3’ m’c

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. \[(1) \quad 1 \quad (0,0,0)\]
2. \[(2) \quad 2 \quad 0,0,z \quad (2_2, 0,0,0)\]
3. \[(3) \quad 4^+ \quad (0,0,1/2) \quad 0,0,z \quad (4_4,0,0,1/2)\]
4. \[(4) \quad 4^+ \quad (0,0,1/2) \quad 0,0,z \quad (4_2^-1,0,0,1/2)\]
5. \[(5) \quad m' \quad x,0,z \quad (m_y,0,0,0)\]
6. \[(6) \quad m' \quad 0,y,z \quad (m_x,0,0,0)\]
7. \[(7) \quad c \quad (0,0,1/2) \quad x,x,z \quad (m_{xy},0,0,1/2)\]
8. \[(8) \quad c \quad (0,0,1/2) \quad x,x,z \quad (m_{xy},0,0,1/2)\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z+1/2 [v,u,w] (4) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 e .m'</td>
<td>x,1/2,z [u,0,w] x,1/2,z [u,0,w] 1/2,x,z+1/2 [0,u,w] 1/2,x,z+1/2 [0,u,w]</td>
</tr>
<tr>
<td>4 d .m'</td>
<td>x,0,z [u,0,w] x,0,z [u,0,w] 0,x,z+1/2 [0,u,w] 0,x,z+1/2 [0,u,w]</td>
</tr>
<tr>
<td>2 c 2m'm'</td>
<td>0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 2m'm'</td>
<td>1/2,1/2,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 2m'm'</td>
<td>0,0,z [0,0,w] 0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'm'm
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p1m'1
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p2\(\bar{1}\)m'1
\[ a^* = -(a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0

105.3.873 - 2 - 1740
Origin on 2mm on 42' mc'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

1. \[ 1 \]
2. \[ 2 0,0,z \]
3. \[ 4^+ \cdot (0,0,1/2) 0,0,z \]
4. \[ 4^- \cdot (0,0,1/2) 0,0,z \]
5. \[ m x,0,z \]
6. \[ m 0,y,z \]
7. \[ c' (0,0,1/2) x,x,z \]
8. \[ c' (0,0,1/2) x,x,z \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<tr>
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<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+1/2 [v,u,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

| 4 e .m. | x,1/2,z [0,v,0] |
|         | x,1/2,z [0,v,0] |
|         | 1/2,x,z+1/2 [v,0,0] |
|         | 1/2,x,z+1/2 [v,0,0] |

| 4 d .m. | x,0,z [0,v,0] |
|         | x,0,z [0,v,0] |
|         | 0,x,z+1/2 [v,0,0] |
|         | 0,x,z+1/2 [v,0,0] |

| 2 c 2mm. | 0,1/2,z [0,0,0] |
|          | 1/2,0,z+1/2 [0,0,0] |

| 2 b 2mm. | 1/2,1/2,z [0,0,0] |
|          | 1/2,1/2,z+1/2 [0,0,0] |

| 2 a 2mm. | 0,0,z [0,0,0] |
|          | 0,0,z+1/2 [0,0,0] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a \ b* = b</td>
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<tr>
<td>Origin at 0,0,z</td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b \ b* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,0</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p1m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2 \ b* = c/2</td>
<td></td>
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<tr>
<td>Origin at x,x,0</td>
<td></td>
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</tbody>
</table>
P4₂ m'c'
105.5.875
Tetragonal

4m'm'
P4₂ m'c'

\[ \text{Origin on } 2m'm' \text{ on } 4₂ m'c' \]

\[ \text{Asymmetric unit} \quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

\[ \text{Symmetry Operations} \]

(1) 1
(1) 0,0,0
(2) 2 0,0,z
(2z) 0,0,0
(3) 4⁺ (0,0,1/2) 0,0,z
(4z) 0,0,1/2
(4) 4⁻ (0,0,1/2) 0,0,z
(4z⁻¹) 0,0,1/2

(5) m' x,0,z
(m_y 0,0,0)'
(6) m' 0,y,z
(m_x 0,0,0)'
(7) c' (0,0,1/2) x,x,z
(m_x 0,0,1/2)'
(8) c' (0,0,1/2) x,x,z
(m_y 0,0,1/2)'
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 f</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
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<td>(6) x,y,z [u,v,w]</td>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
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<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 e</td>
<td>.m' x,1/2,z [u,0,w]</td>
</tr>
<tr>
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<td>x,1/2,z [u,0,w]</td>
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<td>1/2,x,z+1/2 [0,u,w]</td>
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<tr>
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<td>1/2,x,z+1/2 [0,u,w]</td>
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<tr>
<td>4 d</td>
<td>.m' x,0,z [u,0,w]</td>
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<tr>
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<td>x,0,z [u,0,w]</td>
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<td>0,x,z+1/2 [0,u,w]</td>
</tr>
<tr>
<td></td>
<td>0,x,z+1/2 [0,u,w]</td>
</tr>
<tr>
<td>2 c</td>
<td>2m'2m'. 0,1/2,z [0,0,w]</td>
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<tr>
<td></td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b</td>
<td>2m'2m'. 1/2,1/2,z [0,0,w]</td>
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<tr>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a</td>
<td>2m'2m'. 0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4/m'2m' Along [1,0,0] p1m'1
\( a^* = a \) \( b^* = b \)
Origin at 0,0,z

Along [1,1,0] p1m'1
\( a^* = b \) \( b^* = c \)
Origin at x,0,0

\( a^* = (\frac{-a+b}{2}) \) \( b^* = \frac{c}{2} \)
Origin at x,x,0
Origin on 2mm on 4\(_2\)mc

Asymmetric unit \(0 \leq x \leq 1/2;\quad 0 \leq y \leq 1/2;\quad 0 \leq z \leq 1/2\)

Symmetry Operations

For \((0,0,0)\) + set

1. \((1)\) \((1)\) \([0,0,0]\)
2. \((2)\) \(0,0,z\)
   \(\left(2_z\right)0,0,0\)
3. \((3)\) \(4^+ (0,0,1/2) 0,0,z\)
   \(\left(4_z\right)0,0,1/2\)
4. \((4)\) \(4^- (0,0,1/2) 0,0,z\)
   \(\left(4_z^{-1}\right)0,0,1/2\)
5. \((5)\) \(m \times 0,0,0\)
   \(m_y\) \(0,0,0\)
6. \((6)\) \(m \times 0,y,z\)
   \(m_x\) \(0,0,0\)
7. \((7)\) \(c (0,0,1/2) x,x,z\)
   \(m_{xy}\) \(0,0,1/2\)
8. \((8)\) \(c (0,0,1/2) x,x,z\)
   \(m_{xy}\) \(0,0,1/2\)

For \((1,0,0)\) + set

1. \((1)\) \((1)\) \((1,0,0)\)
2. \((2)\) \(1/2,0,z\)
   \(\left(2_z\right)1,0,0\)
3. \((3)\) \(4^+ (0,0,1/2) 1/2,1/2,z\)
   \(\left(4_z\right)1,0,1/2\)
4. \((4)\) \(4^- (0,0,1/2) 1/2,1/2,z\)
   \(\left(4_z^{-1}\right)1,0,1/2\)
5. \((5)\) \((5)\) \((1,0,0)\)
   \(m_y\) \((1,0,0)\)
6. \((6)\) \(1/2,y,z\)
   \(m_x\) \(1,0,0\)
7. \((7)\) \(n (1/2,-1/2,1/2) x+1/2,x,z\)
   \(m_{xy}\) \(1,0,1/2\)
8. \((8)\) \(n (1/2,1/2,1/2) x+1/2,x,z\)
   \(m_{xy}\) \(1,0,1/2\)
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>16 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x',y',z' [u',v',w']</td>
</tr>
<tr>
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<td>(3) y',x',z'+1/2 [v',u',w']</td>
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<td></td>
<td>(4) y,x',z'+1/2 [v,u,w]</td>
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<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x',y',z' [u',v',w']</td>
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<td>(7) y',x',z'+1/2 [v',u',w']</td>
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<td>(8) y,x,z'+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8 e .m'.</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>x',1/2,z' [u,0,w']</td>
</tr>
<tr>
<td>8 d .m.</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td></td>
<td>x',0,z' [0,v',0]</td>
</tr>
<tr>
<td>4 c 2'mm'.</td>
<td>0,1/2,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z'+1/2 [0,u,0]</td>
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<tr>
<td>4 b 2m'm'.</td>
<td>1/2,1/2,z [0,0,w]</td>
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<td>1/2,1/2,z'+1/2 [0,0,w']</td>
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<tr>
<td>4 a 2mm.</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z'+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_m 4mm
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p1m11'
\( a^* = b \quad b^* = c \)
Origin at x,0,0

Along [1,1,0] p_c 1m1
\( a^* = (-a + b)/2 \quad b^* = c/2 \)
Origin at x-1/4,x+1/4,0
**Origin** on 2mm on 4' mc'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1\)
   - \((1)\) \(1\)
   - \((1)\) \((0,0,0)\)

2. \(2\)
   - \((2)\) \(0,0,z\)
   - \((2)\) \((0,0,0)\)

3. \(4\) *' \(0,0,1/2\)
   - \((3)\) \(0,0,z\)
   - \((3)\) \((4,0,0,1/2)\)

4. \(4\) *' \(0,0,1/2\)
   - \((4)\) \(0,0,z\)
   - \((4)\) \((4,0,0,1/2)\)

For \((1,0,0)\) + set

1. \(t'\)
   - \((1)\) \((1,0,0)\)

2. \(2'\)
   - \((2)\) \((1/2,0,z)\)
   - \((2)\) \((1,0,0)\)

3. \(4\) *' \(0,0,1/2\)
   - \((3)\) \((0,1/2,1/2)\)
   - \((3)\) \((1,0,1/2)\)

4. \(4\) *' \(0,0,1/2\)
   - \((4)\) \((1/2,0,1/2)\)
   - \((4)\) \((1,0,1/2)\)

For \((1,0,0)\) *' set

1. \(a'\)
   - \((5)\) \((1,0,0)\)
   - \((5)\) \((0,0,0)\)

2. \(m'\)
   - \((6)\) \((1/2,y,z)\)
   - \((6)\) \((1,0,0)\)

3. \(n\)
   - \((7)\) \((1/2,-1/2,1/2)\)
   - \((7)\) \((1,0,1/2)\)

4. \(n\)
   - \((8)\) \((1/2,1/2,1/2)\)
   - \((8)\) \((1,0,1/2)\)
Generators selected  
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>16 f 1</td>
<td>(0,0,0) +</td>
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<tr>
<td>15 g 1</td>
<td>(1,0,0) +</td>
</tr>
<tr>
<td>8 e .m'.</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 d .m.</td>
<td>(2) x',y',z'[u',v',w']</td>
</tr>
<tr>
<td>4 c 2'mm'</td>
<td>(3) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 b 2m'm'</td>
<td>(4) y',x',z+1/2 [v',u',w']</td>
</tr>
<tr>
<td>4 a 2mm.</td>
<td>(5) x',y',z'[u',v',w']</td>
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<tr>
<td></td>
<td>(6) x',y',z'[u',v',w']</td>
</tr>
<tr>
<td></td>
<td>(7) y',x',z+1/2 [v',u',w']</td>
</tr>
<tr>
<td></td>
<td>(8) y',x',z+1/2 [v',u',w']</td>
</tr>
<tr>
<td></td>
<td>(9) x',y',z'[u',v',w']</td>
</tr>
<tr>
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<td>(10) y',x',z+1/2 [v',u',w']</td>
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<tr>
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<td>(11) x',y',z'[u',v',w']</td>
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<tr>
<td></td>
<td>(12) y',x',z+1/2 [v',u',w']</td>
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<td>(13) x',y',z'[u',v',w']</td>
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<tr>
<td></td>
<td>(14) y',x',z+1/2 [v',u',w']</td>
</tr>
<tr>
<td></td>
<td>(15) x',y',z'[u',v',w']</td>
</tr>
<tr>
<td></td>
<td>(16) y',x',z+1/2 [v',u',w']</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{4c}4mm'  
| a' = a | b' = b |
| Origin at 0,0,z |

Along [1,0,0] p1m11'  
| a' = b | b* = c |
| Origin at x,0,0 |

Along [1,1,0] p_{2c}1m1  
| a' = (a + b)/2 | b* = c/2 |
| Origin at x+1/4,x+1/4,0 |
Origin on 2 on $4_2\overline{1}n$

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$
(1) $1$

(2) $2 \ 0,0,z$
(2) $z \ 0,0,z$

(3) $4^+ (0,0,1/2) \ 0,0,z$
(3) $4 \ 0,0,1/2$

(4) $4^- (0,0,1/2) \ 0,0,z$
(4) $4^- \ 0,0,1/2$

(5) a $(1/2,0,0) \ x,1/4,z$
(5) x,1/4,z

(6) b $(0,1/2,0) \ 1/4,y,z$
(6) $1/4,y,z$

(7) c $(0,0,1/2) \ x+1/2,x,z$
(7) $1/2,1/2,z$

(8) n $(1/2,1/2,1/2) \ x,x,z$
(8) $1/2,1/2,x$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z+1/2 [v,u,w]</td>
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<tr>
<td></td>
<td>(4) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<tr>
<td>4 b 2..</td>
<td>0,1/2,z [0,0,w]</td>
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<td>1/2,0,z+1/2 [0,0,w]</td>
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<td>4 a 2..</td>
<td>0,0,z [0,0,w]</td>
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<td>0,0,z+1/2 [0,0,w]</td>
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<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm

\[
\begin{align*}
\mathbf{a}^* &= \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \\
\text{Origin at 0,0,z}
\end{align*}
\]

Along [1,0,0] \( p_{2a'1m1} \)

\[
\begin{align*}
\mathbf{a}^* &= \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c} \\
\text{Origin at x,1/4,0}
\end{align*}
\]

Along [1,1,0] \( p_{2b'1m'1} \)

\[
\begin{align*}
\mathbf{a}^* &= (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \\
\text{Origin at x,x,0}
\end{align*}
\]
Origin on 21' on 4_2 1n1'

Asymmetric unit  
0 ≤ x ≤ 1/2;  
0 ≤ y ≤ 1/2;  
0 ≤ z ≤ 1/2

Symmetry Operations

For 1 + set

(1) 1  
(1 | 0, 0, 0)

(5) a (1/2, 0, 0)  x 1/4, z  
(m_y | 1/2, 1/2, 0)

(2) 2  0, 0, z  
(2_z | 0, 0, 0)

(6) b (0, 1/2, 0)  1/4, y, z  
(m_x | 1/2, 1/2, 0)

(3) 4^+ (0, 0, 1/2)  0, 0, z  
(4_z | 0, 0, 1/2)

(7) c (0, 0, 1/2)  x+1/2, x, z  
(m_x | 1/2, 1/2, 1/2)

(4) 4^*- (0, 0, 1/2)  0, 0, z  
(4_z^- | 0, 0, 1/2)

For 1' + set

(1) 1'  
(1 | 0, 0, 0)'

(5) a' (1/2, 0, 0)  x 1/4, z  
(m_y | 1/2, 1/2, 0)'

(2) 2'  0, 0, z  
(2_z | 0, 0, 0)'

(6) b' (0, 1/2, 0)  1/4, y, z  
(m_x | 1/2, 1/2, 0)'

(3) 4^+* (0, 0, 1/2)  0, 0, z  
(4_z | 0, 0, 1/2)'

(7) c' (0, 0, 1/2)  x+1/2, x, z  
(m_x | 1/2, 1/2, 1/2)'

(4) 4^-* (0, 0, 1/2)  0, 0, z  
(4_z^- | 0, 0, 1/2)'

(8) n' (1/2, 1/2, 1/2)  x, x, z  
(m_x | 1/2, 1/2, 1/2)'

106.2.879 - 1 - 1751
Generators selected

$(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'$.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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</tr>
</thead>
<tbody>
<tr>
<td>1 +</td>
<td>1' +</td>
</tr>
</tbody>
</table>

| 8  | c  | 11' | 1) x,y,z [0,0,0] | (2) x,y,z [0,0,0] |
| 3  | y+1/2,x+1/2,z [0,0,0] | (4) y,x,z+1/2 [0,0,0] |
| 4  | b  | 2..1' | 0,1/2,z [0,0,0] | 1/2,0,z+1/2 [0,0,0] |
| 4  | a  | 2..1' | 0,0,z [0,0,0] | 0,0,z+1/2 [0,0,0] |
| 4  | b  | 2..1' | 0,1/2,z [0,0,0] | 0,0,z+1/2 [0,0,0] |
| 4  | a  | 2..1' | 1/2,0,z [0,0,0] | 0,1/2,z+1/2 [0,0,0] |
| 4  | a  | 2..1' | 1/2,1/2,z+1/2 [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4gm1'</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [1,1,0]</th>
<th>p1m11'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Origin on 2 on 4\_2\_1n**

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

1. (1) \[ 1 \]
   \[ (1/0,0,0) \]

2. (2) \[ z \]
   \[ (2z/0,0,0) \]

3. (3) \[ 4\_z^+ (0,0,1/2) 0,0,z \]
   \[ (4z/0,0,1/2) \]

4. (4) \[ 4\_z^- (0,0,1/2) 0,0,z \]
   \[ (4z^-/0,0,1/2) \]

5. (5) \[ a\_x' (1/2,0,0) x,1/4,z \]
   \[ (m\_y/1/2,1/2,0) \]

6. (6) \[ b' (0,1/2,0) 1/4,y,z \]
   \[ (m\_x/1/2,1/2,0) \]

7. (7) \[ c (0,0,1/2) x+1/2,1/4,z \]
   \[ (m\_y/1/2,1/2,1/2) \]

8. (8) \[ n (1/2,1/2,1/2) x,x,z \]
   \[ (m\_x/1/2,1/2,1/2) \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x ,y ,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y' ,x,z+1/2 [v,u,w]</td>
</tr>
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<td></td>
<td>(4) y, x,z+1/2 [v,u,w]</td>
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<tr>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y'+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 b 2..</td>
<td>0,1/2,z [0,0,w]</td>
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<tr>
<td></td>
<td>1/2,0,z+1/2 [0,0,w]</td>
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<td>1/2,0,z [0,0,w]</td>
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<td>0,1/2,z+1/2 [0,0,w]</td>
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<td>4 a 2..</td>
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<td>0,0,z+1/2 [0,0,w]</td>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4g'm

\( a^* = a \quad b^* = b \)

Origin at 0,0,z

Along [1,0,0] p1m'1

\( a^* = b/2 \quad b^* = c \)

Origin at x,0,0

Along [1,1,0] p2v',1m'1

\( a^* = (-a + b)/2 \quad b^* = c/2 \)

Origin at x,x,0
Origin on $4'_{2}, 1n'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$

(2) $2 \quad 0,0,0$

(5) $a\ (1/2,0,0)\ x,1/4,z$

(6) $b\ (0,1/2,0)\ 1/4,y,z$

(7) $c'\ (0,0,1/2)\ x+1/2,x,z$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>8</td>
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<td>(1) x,y,z [u,v,w]</td>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z+1/2 [v,u,w]</td>
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<td>(4) y,x,z+1/2 [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
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<td></td>
<td></td>
<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1] p4'gm'**  
  - $a^* = a$  
  - $b^* = b$
  - Origin at 0,0,z

- **Along [1,0,0] p2a*1m1**  
  - $a^* = b/2$  
  - $b^* = c$
  - Origin at x,1/4,0

- **Along [1,1,0] p1m'1**  
  - $a^* = (a + b)/2$  
  - $b^* = c/2$
  - Origin at x,x,0
P4₂ b'c'  4m'm'  Tetragonal

106.5.882  P4₂ b'c'

Origin on 2  on 4₂ 1n'

Asymmetric unit  
\[0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}\]

Symmetry Operations

1. 1
   
   \[(1) 0,0,0\]

2. 2 0,0,z
   \[(2) z,0,0,0\]

3. 4⁺ (0,0,1/2) 0,0,z
   \[(3) z,0,0,1/2\]

4. 4⁻ (0,0,1/2) 0,0,z
   \[(4) z,0,0,1/2\]

5. a' (1/2,0,0) x,1/4,z
   \[(5) m,1/2,1/2,0'\]

6. b' (0,1/2,0) 1/4,y,z
   \[(6) m,1/2,1/2,0'\]

7. c' (0,0,1/2) x+1/2,x,z
   \[(7) m,1/2,1/2,1/2'\]

8. n' (1/2,1/2,1/2) x,x,z
   \[(8) m,1/2,1/2,1/2'\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<tr>
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<tbody>
<tr>
<td>8</td>
<td>c 1</td>
</tr>
</tbody>
</table>

(1) x,y,z [u,v,w]

(2) x,y,z [u,v,w]

(3) y,x,z+1/2 [v,u,w]

(4) y,x,z+1/2 [v,u,w]

(5) x+1/2, y+1/2, z [u,v,w]

(6) x+1/2, y+1/2, z [u,v,w]

(7) y+1/2, x+1/2, z+1/2 [v,u,w]

(8) y+1/2, x+1/2, z+1/2 [v,u,w]

4 b 2.. 0,1/2,z [0,0,w]

1/2,0,z+1/2 [0,0,w]

1/2,0,z [0,0,w]

0,1/2,z+1/2 [0,0,w]

4 a 2.. 0,0,z [0,0,w]

0,0,z+1/2 [0,0,w]

1/2,1/2,z [0,0,w]

1/2,1/2,z+1/2 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p4g’m’

A* = a  b* = b

Origin at 0,0,z

Along [1,0,0] p1m’1

A* = b/2  b* = c

Origin at x,0,0

Along [1,1,0] p1m’1

A* = (-a + b)/2  b* = c/2

Origin at x,x,0
I4mm 4mm Tetragonal

107.1.883

Origin on 4mm

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

For $(0,0,0) + set$

1. $I \quad 0,0,0$
2. $2 \quad 0,0,z \quad (2z,0,0,0)$
3. $4^+ \quad 0,0,z \quad (4z,0,0,0)$
4. $4^- \quad 0,0,z \quad (4z^{-1},0,0,0)$
5. $m \quad x,0,z \quad (m_y,0,0,0)$
6. $m \quad 0,y,z \quad (m_x,0,0,0)$
7. $m \quad x,x,z \quad (m_{xy},0,0,0)$
8. $m \quad x,x,z \quad (m_{xy},0,0,0)$

For $(1/2,1/2,1/2) + set$

1. $t \quad (1/2,1/2,1/2) \quad 1/4,1/4,z \quad (2z,1/2,1/2,1/2)$
2. $2 \quad (0,0,1/2) \quad 0,1/2,z \quad (4z^{-1},1/2,1/2,1/2)$
3. $4^+ \quad (0,0,1/2) \quad 0,1/2,z \quad (4z^{-1},1/2,1/2,1/2)$
4. $4^- \quad (0,0,1/2) \quad 1/2,0,z \quad (4z^{-1},1/2,1/2,1/2)$
5. $n \quad (1/2,0,1/2) \quad x,1/4,z \quad (m_y,1/2,1/2,1/2)$
6. $n \quad (0,1/2,1/2) \quad 1/4,y,z \quad (m_x,1/2,1/2,1/2)$
7. $c \quad (0,0,1/2) \quad x+1/2,x,z \quad (m_{xy},1/2,1/2,1/2)$
8. $n \quad (1/2,1/2,1/2) \quad x,x,z \quad (m_{xy},1/2,1/2,1/2)$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 e 1</td>
<td>(1) x,y,z [u,v,w] (2) x' y' z [u',v',w'] (3) y' x' z [v,u,w] (4) y' x' z [v,u,w]</td>
</tr>
<tr>
<td>8 d .m.</td>
<td>x,0,z [0,v,0] x' ,0,z [0,v',0] 0,x,z [v,0,0] 0,x,z [v,0,0]</td>
</tr>
<tr>
<td>8 c .m.</td>
<td>x,x,z [u,u,0] x' ,x,z [u',u,0] 0,x,z [v,0,0] 0,x,z [u,0,0]</td>
</tr>
<tr>
<td>4  b 2mm.</td>
<td>0,1/2,z [0,0,0] 1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2  a 4mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm
a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] c1m1
a* = b  b* = c
Origin at x,0,0

Along [1,1,0] p1m11'
a* = (-a + b)/2  b* = c/2
Origin at x,x,0
**Origin** on 4mm1'

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \((1) 1\)
   - \((1) 0,0,0\)
2. \((2) 2 0,0,z\)
   - \((2_z, 0,0,0)\)
3. \((3) 4^+ 0,0,z\)
   - \((4_z, 0,0,0)\)
4. \((4) 4^- 0,0,z\)
   - \((4_z^{-1}, 0,0,0)\)

5. \((5) m x,0,z\)
   - \((m, x,0,0,0)\)
6. \((6) m 0,y,z\)
   - \((m, 0,y,0,0)\)
7. \((7) m x,x,z\)
   - \((m_{xy}, x,x,0,0)\)
8. \((8) m x,x,z\)
   - \((m_{xy}, x,x,0,0)\)

For \((1/2,1/2,1/2) + \text{set}\)

1. \((1) t (1/2,1/2,1/2)\)
   - \((1/2,1/2,1/2)\)
2. \((2) 2 (0,0,1/2) 1/4,1/4,z\)
   - \((2_z, 1/2,1/2,1/2)\)
3. \((3) 4^+ (0,0,1/2) 0,1/2,z\)
   - \((4_z, 1/2,1/2,1/2)\)
4. \((4) 4^- (0,0,1/2) 1/2,0,z\)
   - \((4_z^{-1}, 1/2,1/2,1/2)\)

5. \((5) n (1/2,0,1/2) x,1/4,z\)
   - \((m, 1/2,0,1/2)\)
6. \((6) n (0,1/2,1/2) 1/4,y,z\)
   - \((m, 1/2,1/2,1/2)\)
7. \((7) c (0,0,1/2) x+1/2,x,z\)
   - \((m_{xy}, x+1/2,x,0,0)\)
8. \((8) n (1/2,1/2,1/2) x,x,z\)
   - \((m_{xy}, x,x,0,0)\)
Continued

For (0,0,0)'+ set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t'</td>
<td>(0,0,0)</td>
<td>e, [0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(2) 2'</td>
<td>(0,0,0)</td>
<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(3) 4'</td>
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<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
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<tr>
<td>(4) 4'</td>
<td>(0,0,0)</td>
<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
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</table>

For (1/2,1/2,1/2)'+ set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5) n'</td>
<td>(0,0,0)</td>
<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(6) n'</td>
<td>(0,0,0)</td>
<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
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<tr>
<td>(7) n'</td>
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<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(8) n'</td>
<td>(0,0,0)</td>
<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
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</tbody>
</table>

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

### Positions

<table>
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<th>Site Symmetry</th>
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<tbody>
<tr>
<td>16 e</td>
<td>(0,0,0)</td>
<td>[0,0,0]</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
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<tr>
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<td>(1/2,1/2,1/2)'+</td>
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<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
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<td>4 b</td>
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<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2)</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>c1m11'</th>
<th>Along [1,1,0]</th>
<th>p1m11'</th>
</tr>
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<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -(a + b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

107.2.884 - 2 - 1762
I4'm'm
107.3.885

I4'm'm

Tetragonal

Origin on 4'm'm

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1; \quad x < y \]

Symmetry Operations

For (0,0,0) + set

1. \(1\)
   \(1\left|0,0,0\right)\)
2. \(2\)
   \(0,0,z\)
   \(2_z\left|0,0,0\right)\)
3. \(4^+\) \(0,0,z\)
   \(4_z\left|0,0,0\right)\)
4. \(4^-\) \(0,0,z\)
   \(4_z^{-1}\left|0,0,0\right)\)
5. \(m'\) \(x,0,z\)
   \(m_y\left|x,0,0\right)\)
6. \(m'\) \(0,y,z\)
   \(m_x\left|0,0,0\right)\)
7. \(m\) \(x,x,z\)
   \(m_{xy}\left|x,0,0\right)\)
8. \(m\) \(x,x,z\)
   \(m_{xy}\left|0,0,0\right)\)

For (1/2,1/2,1/2) + set

1. \(t\) \(1/2,1/2,1/2\)
   \(1\left|1/2,1/2,1/2\right)\)
2. \(2\)
   \(0,0,1/2\)
   \(1/4,1/4,z\)
   \(2_z\left|1/2,1/2,1/2\right)\)
3. \(4^+\) \(0,0,1/2\)
   \(0,1/2,z\)
   \(4_z\left|1/2,1/2,1/2\right)\)
4. \(4^-\) \(0,0,1/2\)
   \(1/2,0,z\)
   \(4_z^{-1}\left|1/2,1/2,1/2\right)\)
5. \(n'\) \(1/2,0,1/2\)
   \(x,1/4,z\)
   \(m_y\left|1/2,1/2,1/2\right)\)
6. \(n'\) \(0,1/2,1/2\)
   \(1/4,y,z\)
   \(m_x\left|1/2,1/2,1/2\right)\)
7. \(c\) \(0,0,1/2\)
   \(x+1/2,x,z\)
   \(m_{xy}\left|1/2,1/2,1/2\right)\)
8. \(n\) \(1/2,1/2,1/2\)
   \(x,x,z\)
   \(m_{xy}\left|1/2,1/2,1/2\right)\)
Continued

### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
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<td>8 d .m'</td>
<td>x,0,z [u,0,w]</td>
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<tr>
<td>2 a 4'm'm</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p4mm'
  - \( a^* = (a - b)/2 \)
  - \( b^* = (a + b)/2 \)
- **Along [1,0,0]**: c1m'
  - \( a^* = b \)
  - \( b^* = c \)
- **Along [1,1,0]**: p1m1'
  - \( a^* = (-a + b)/2 \)
  - \( b^* = c/2 \)

Origin at 0,0,z
Origin at x,0,0
Origin at x,x,0
**Origin** on 4'\textit{mm}'

**Asymmetric unit** \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\)

**Symmetry Operations**

For \((0,0,0) + \text{set}\):

1. \(1 \quad (1)\) 0,0,0
2. \(2 \quad (2)\) 0,0,z
   \((2_2)\) 0,0,0
3. \(4^+ \quad (3)\) 0,0,z
   \((4_z)\) 0,0,0,'
4. \(4^- \quad (4)\) 0,0,z
   \((4_z^{-1})\) 0,0,0,'
5. \(m \quad (5)\) x,0,z
   \((m_y)\) 0,0,0
6. \(m \quad (6)\) 0,y,z
   \((m_x)\) 0,0,0
7. \(m' \quad (7)\) x,x,z
   \((m_{xy})\) 0,0,0,'
8. \(m' \quad (8)\) x,x,z
   \((m_{xy})\) 0,0,0,'

For \((1/2,1/2,1/2) + \text{set}\):

1. \(t \quad (1)\) 1/2,1/2,1/2
   \((1)\) 1/2,1/2,1/2
2. \(2 \quad (2)\) 0,0,1/2
   \((2_z)\) 1/2,1/2,1/2
3. \(4^+ \quad (3)\) 0,0,1/2
   \((4_z)\) 1/2,1/2,1/2,'
4. \(4^- \quad (4)\) 0,0,1/2
   \((4_z^{-1})\) 1/2,1/2,1/2,'
5. \(n \quad (5)\) x,1/4,z
   \((m_x)\) 1/2,1/2,1/2
6. \(n \quad (6)\) 0,1/2,1/2
   \((m_x)\) 1/2,1/2,1/2
7. \(c' \quad (7)\) 0,0,1/2
   \((m_{xy})\) 1/2,1/2,1/2,'
8. \(n' \quad (8)\) x,1/2,1/2
   \((m_{xy})\) 1/2,1/2,1/2,'
Generators selected

$(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5)$.

Positions

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<tr>
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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<tbody>
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<td>(1/2,1/2,1/2) +</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>2</td>
<td>a</td>
<td>0,0,z [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along $[0,0,1]$ p4'm'm

$ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2$

Origin at 0,0,z

Along $[1,0,0]$ c1m11'

$ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}$

Origin at x,0,0

Along $[1,1,0]$ p1m1'

$ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2$

Origin at x,x,0
**Tetragonal**  
107.5.887

**Symmetry Operations**

For (0,0,0) + set

1. 1
   
2. $2 \cdot 0,0,z$
   
3. $4^+ \cdot 0,0,z$
   
4. $4^* \cdot 0,0,z$

(1)* $0,0,0$

(2)* $z,0,0,0$

(3)* $4,0,0,0$

(4)* $4^*,-1,0,0,0$

5. $m',x,0,z$
   
6. $m',0,y,z$
   
7. $m',0,x,z$
   
8. $m',x,x,z$

For (1/2,1/2,1/2) + set

1. $t \cdot 1/2,1/2,1/2$
   
2. $2 \cdot (0,0,1/2),1/4,1/4,z$
   
3. $4^+ \cdot (0,0,1/2),1/2,1/2,1/2$ (2)* $z,1/2,1/2,1/2$

4. $4^* \cdot (0,0,1/2),1/2,1/2,1/2$

(1)* $1/2,1/2,1/2$

(2)* $z,1/2,1/2,1/2$

(3)* $z,1/2,1/2,1/2$

(4)* $1/2,1/2,1/2$

5. $n' \cdot 1/2,0,1/2,x,1/4,z$
   
6. $n' \cdot (0,1/2,1/2),1/4,y,z$
   
7. $c' \cdot (0,0,1/2),x+1/2,x$, $z$
   
8. $n' \cdot (1/2,1/2,1/2),x,x,z$

(5)* $1/2,1/2,1/2$

(6)* $z,1/2,1/2,1/2$

(7)* $z,1/2,1/2,1/2$

(8)* $1/2,1/2,1/2$
Continued

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

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<tbody>
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<tr>
<td>16 e</td>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4m’m’</td>
</tr>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
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<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,0,0]</td>
<td>c1m’1</td>
</tr>
<tr>
<td>a* = b</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
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</tbody>
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<tr>
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<th>Symmetry</th>
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<tbody>
<tr>
<td>Along [1,1,0]</td>
<td>p1m’1</td>
</tr>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
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</tbody>
</table>
Origin on 4mm

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\)

Symmetry Operations

For \((0,0,0) + \) set

1. \((1) 1\)
   \(1) 0,0,0\)

5. \((5) m \ x,0,z\)
   \((m_y|0,0,0)\)

For \((1/2,1/2,1/2)^* + \) set

1. \((1) t' (1/2,1/2,1/2)^*\)

3. \((3) 4^* (0,0,1/2) \ 0,1/2,z\)
   \((4^*|1/2,1/2,1/2)^*\)

5. \((5) n' (1/2,0,1/2) \ x,1/4,z\)
   \((m_y|1/2,1/2,1/2)^*\)

7. \((7) c' (0,0,1/2) \ x+1/2,1/2,z\)
   \((m_{xy}|1/2,1/2,1/2)^*\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<tr>
<td></td>
<td>(1/2,1/2,1/2)’ +</td>
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<td>(0,0,0), x,y,z [u,v,w]</td>
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<td>x,0,z [0,v,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_4, 4mm</th>
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</thead>
<tbody>
<tr>
<td>a^* = (a - b)/2</td>
<td>b^* = (a + b)/2</td>
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<table>
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<th>Along [1,0,0]</th>
<th>c1m11’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = b</td>
<td>b^* = c</td>
</tr>
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</tbody>
</table>

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<tr>
<th>Along [1,1,0]</th>
<th>p1m11’</th>
</tr>
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<tbody>
<tr>
<td>a^* = -a + b/2</td>
<td>b^* = c/2</td>
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<tr>
<td>Origin at x,x,0</td>
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</tbody>
</table>
Origin on 4'm'm

Asymmetric unit \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1; \ x \leq y \)

Symmetry Operations

For \((0,0,0)\) + set

(1) \(1\)  
(1) \(0,0,0\)

(2) \(2\) 0,0,z  
(2) \(0,0,0\)

(3) \(4^+\) 0,0,z  
(4) \(0,0,0\)

(4) \(4^-\) 0,0,z  
(4) \(0,0,0\)

(5) \(m\) x,0,z  
(5) \(0,0,0\)

(6) \(m'\) 0,y,z  
(6) \(0,0,0\)

(7) \(m\) x,x,z  
(7) \(0,0,0\)

(8) \(m\) x,x,z  
(8) \(0,0,0\)

For \((1/2,1/2,1/2)\) + set

(1) \(t\) (1/2,1/2,1/2)  
(1) \(1/2,1/2,1/2\)

(2) \(2'\) (0,0,1/2)  
(2) \(1/2,1/2,1/2\)

(3) \(4^+\) (0,0,1/2)  
(3) \(1/2,1/2,1/2\)

(4) \(4^-\) (0,0,1/2)  
(4) \(1/2,1/2,1/2\)

(5) \(n\) (1/2,0,1/2)  
(5) \(1/2,1/2,1/2\)

(6) \(n\) (0,1/2,1/2)  
(6) \(1/2,1/2,1/2\)

(7) \(c'\) (0,0,1/2)  
(7) \(1/2,1/2,1/2\)

(8) \(n'\) (1/2,1/2,1/2)  
(8) \(1/2,1/2,1/2\)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

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<td>(5) x',y',z [u',v',w]</td>
</tr>
<tr>
<td></td>
<td>(7) y',x',z [v',u',w]</td>
</tr>
<tr>
<td>8 d m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>8 c m</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>4 b m' m'</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a m' m'</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] \( p_{6} 4m' m' \)

\( a^{*} = (a - b)/2 \) \( b^{*} = (a + b)/2 \)

Origin at 0,1/2,z

Along [1,0,0] \( c_{6} 1m' 1 \)

\( a^{*} = b \) \( b^{*} = c \)

Origin at x,0,0

Along [1,1,0] \( p_{1} m 11' \)

\( a^{*} = (-a + b)/2 \) \( b^{*} = c/2 \)

Origin at x,x,0
Origin on 4'mm'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x < y$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1
   (1) 0,0,0

(2) $2' - 0,0,z$
   (2) $2_{z} - 0,0,0$

(3) $4^{+} - 0,0,z$
   (4) $(4_{z} - 0,0,0)^{'}$

(4) $4^{-} - 0,0,z$
   (4) $(4_{z}^{-1} - 0,0,0)^{'}$

(5) $m - x,0,z$
   (m) $0,y,z$

(6) $m - 0,y,z$
   (6) $m_{x} - 0,0,0$

(7) $m^{'} - x,x,z$
   (7) $m_{x}^{'} - 0,0,0$

(8) $m^{'} - x,x,z$
   (8) $m_{x}^{'} - 0,0,0$

For $(1/2,1/2,1/2)^{'} + set$

(1) $t' - (1/2,1/2,1/2)^{'}$
   (1) $1/2,1/2,1/2$' + set

(2) $2' - (0,0,1/2) - 1/4,1/4,z$
   (2) $2_{z} - 1/2,1/2,1/2$'

(3) $4^{+} - (0,0,1/2) - 0,1/2,z$
   (3) $4_{z} - 1/2,1/2,1/2$

(4) $4^{-} - (0,0,1/2) - 1/2,0,z$
   (4) $(4_{z}^{-1} - 1/2,1/2,1/2)$

(5) $n' - (1/2,0,1/2) - x,1/4,z$
   (5) $1/2,1/2,1/2$'

(6) $n' - (0,1/2,1/2) - 1/4,y,z$
   (6) $(m_{x} - 1/2,1/2,1/2)^{'}$

(7) $c - (0,0,1/2) - x+1/2, x,z$
   (7) $(m_{x} - 1/2,1/2,1/2)^{'}$

(8) $n - (1/2,1/2,1/2) - x,x,z$
   (8) $(m_{x} - 1/2,1/2,1/2)^{'}$
Generators selected

\[(1); t(1,0,0); t(0,1,0); t'(1/2,1/2,1/2); (2); (3); (5).\]

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
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<td>16 e 1</td>
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<tr>
<td></td>
<td>(1/2,1/2,1/2)′ +</td>
</tr>
<tr>
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<td>(2) x, y,z [u, v, w]</td>
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<td>(5) x, y,z [u, v, w]</td>
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<td>0,0,z [0,0,0]</td>
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<tr>
<td></td>
<td>x,0,z [0, v, 0]</td>
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<td>8 c.m.’</td>
<td>x,x,z [u,u,w]</td>
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<td>4 b 2mm.</td>
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</tr>
<tr>
<td>2 a 4’mm’</td>
<td>0,0,z [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{6}^{4},4 \text{mm} \) \( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \) \( \text{Origin at } 0,1/2,z \)
Along [1,0,0] \( c1\text{m}11' \) \( a^* = b \) \( b^* = c \) \( \text{Origin at x,0,0} \)
Along [1,1,0] \( p_{2}^{21},1 \text{m}1' \) \( a^* = (a - b)/2 \) \( b^* = c/2 \) \( \text{Origin at x,x,0} \)
Tetragonal

IP 4mm'

107.9.891

Tetragonal

Origin on 4mm'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1; \ x < y \]

Symmetry Operations

For \((0,0,0)\) + set

1. \((1, 0, 0, 0)\)
2. \((2, 0, 0, z)\)
3. \((3, 4, 0, 0, z)\)
4. \((4, 4, -1, 0, 0, z)\)

5. \((5, m', x, 0, z)\)
6. \((6, m', 0, y, z)\)
7. \((7, m', x, x, z)\)
8. \((8, m', x, x, z)\)

For \((1/2,1/2,1/2)\)' + set

1. \((1, 1/2, 1/2, 1/2)\')
2. \((2, 0, 0, 1/2)\) \((1/4, 1/4, 1/4, z)\)
3. \((3, 4, 0, 0, 1/2)\) \((0, 1/2, 1/2, 1/2)\)
4. \((4, 4, -1, 0, 0, 1/2)\) \((1/2, 1/2, 1/2, 1/2)\)

5. \((5, n, x, 1/4, z)\)
6. \((6, n, 0, 1/2, 1/2)\) \((1/4, y, z)\)
7. \((7, c, (0, 0, 1/2)\) \((x+1/2, x, z)\)
8. \((8, n, (1/2, 1/2, 1/2)\) \((x, x, z)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>x,0,z [u,0,w]</td>
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<td>8 c .m’</td>
<td>x,x,z [u,u,w]</td>
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<tr>
<td>4 b 2m’m’</td>
<td>0,1/2,z [0,0,w]</td>
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<tr>
<td>2 a 4m’m’</td>
<td>0,0,z [0,0,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{a’} \) 4m’m’

\( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)

Origin at 0,0,z

Along [1,0,0] \( c_{p,1} \) m’1

\( a^* = b \) \( b^* = c \)

Origin at x,0,0

Along [1,1,0] \( p_{2b} \) 1m’1

\( a^* = (-a + b)/2 \) \( b^* = c/2 \)

Origin at x,x,0
**Symmetry Operations**

**For (0,0,0) + set**

1. \(1 \quad 1\)
2. \(2 \quad 0,0,z\)
3. \(4^+ \quad 0,0,z\)
4. \(4^- \quad 0,0,z\)
5. \(a \quad (1/2,0,0)\)
6. \(b \quad (0,1/2,0)\)
7. \(m \quad x+1/2, \bar{x}, z\)
8. \(g \quad (1/2,1/2,0)\)

**For (1/2,1/2,1/2) + set**

1. \(t \quad (1/2,1/2,1/2)\)
2. \(2 \quad (0,0,1/2)\)
3. \(4^+ \quad (0,0,1/2)\)
4. \(4^- \quad (0,0,1/2)\)
5. \(c \quad (0,0,1/2)\)
6. \(c \quad (0,0,1/2)\)
7. \(c \quad (0,0,1/2)\)
8. \(c \quad (0,0,1/2)\)

---

**Origin on 4cc**

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>(7) x,y,z [v,u,w]</td>
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<td>(8) x,y,z [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>c</td>
<td>x + 1/2, y + 1/2, z [u, v, w]</td>
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<tr>
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<td>x + 1/2, x + 1/2, z [u, v, w]</td>
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<td>b</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>1/2, 1/2, z [0, 0, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm
a* = (a - b)/2   b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2a1m1
a* = b/2   b* = c/2
Origin at x,1/4,0

Along [1,1,0] p1m11
a* = -(a + b)/2   b* = c/2
Origin at x,x,0
**Origin** on 4cc1’

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x \]

**Symmetry Operations**

For \((0,0,0) +\) set

1. \(1\) \(0,0,0\)
2. \(2\) \(0,0,z\) \((2_z 0,0,0)\)
3. \(4^+\) \(0,0,z\) \((4_z 0,0,0)\)
4. \(4^-\) \(0,0,z\) \((4_z^{-1} 0,0,0)\)
5. \(a\) \((1/2,0,0)\) \(x,0,z\) \((m_y | 1/2,1/2,0)\)
6. \(b\) \((0,1/2,0)\) \(1/4,y,z\) \((m_x | 1/2,1/2,0)\)
7. \(m\) \(x+1/2,x,z\) \((m_x | 1/2,1/2,0)\)
8. \(g\) \((1/2,1/2,0)\) \(x,x,z\) \((m_y | 1/2,1/2,0)\)

For \((1/2,1/2,1/2) +\) set

1. \(t\) \((1/2,1/2,1/2)\)
2. \(2\) \((0,0,1/2)\) \(1/4,1/4,z\) \((2_z | 1/2,1/2,1/2)\)
3. \(4^+\) \((0,0,1/2)\) \(0,1/2,z\) \((4_z | 1/2,1/2,1/2)\)
4. \(4^-\) \((0,0,1/2)\) \(1/2,0,z\) \((4_z^{-1} | 1/2,1/2,1/2)\)
5. \(c\) \((0,0,1/2)\) \(x,0,z\) \((m_y | 0,0,1/2)\)
6. \(c\) \((0,0,1/2)\) \(0,y,z\) \((m_x | 0,0,1/2)\)
7. \(c\) \((0,0,1/2)\) \(x,x,z\) \((m_y | 0,0,1/2)\)
8. \(c\) \((0,0,1/2)\) \(x,x,z\) \((m_y | 0,0,1/2)\)
Continued

For \((0,0,0)\)' + set

1. \(1'\)
   \((1|0,0,0)'\)
2. \(2'\) 0,0,z
   \((2|0,0,0)'\)
3. \(4^* + 0,0,z\)
   \((4|0,0,0)'\)
4. \(4^* - 0,0,z\)
   \((4^{-1}|0,0,0)'\)

(5) \(a' (1/2,0,0) x,1/4,z\)
   \((m_x|1/2,1/2,0)'\)
(6) \(b' (0,1/2,0) 1/4,y,z\)
   \((m_x|1/2,1/2,0)'\)
(7) \(m' x+1/2,x,z\)
   \((m_x|1/2,1/2,0)'\)
(8) \(g' (1/2,1/2,0) x,x,z\)
   \((m_x|1/2,1/2,0)'\)

For \((1/2,1/2,1/2)'\) + set

1. \(t' (1/2,1/2,1/2)\)
   \((1|1/2,1/2,1/2)'\)
2. \(2' (0,0,1/2) 1/4,1/4,z\)
   \((2|1/2,1/2,1/2)'\)
3. \(4^* (0,0,1/2) 0,1/2,z\)
   \((4|1/2,1/2,1/2)'\)
4. \(4^* + 0,0,1/2) 1/2,0,z\)
   \((4^{-1}|1/2,1/2,1/2)'\)

(5) \(c' (0,0,1/2) x,0,z\)
   \((m_x|0,0,1/2)'\)
(6) \(c' (0,0,1/2) 0,y,z\)
   \((m_x|0,0,1/2)'\)
(7) \(c' (0,0,1/2) x,x,z\)
   \((m_x|0,0,1/2)'\)
(8) \(c' (0,0,1/2) x,x,z\)
   \((m_x|0,0,1/2)'\)

Generators selected

(1); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(1/2,1/2,1/2)\); (2); (3); (5); \(1'\).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 d 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) (\bar{x},\bar{y},z [0,0,0])</td>
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<td>(3) (\bar{y},x,z [0,0,0])</td>
<td>(4) y,x,z [0,0,0]</td>
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<td></td>
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<td>(7) (\bar{y}+1/2,\bar{x}+1/2,z [0,0,0])</td>
<td>(8) (y+1/2,x+1/2,z [0,0,0])</td>
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<table>
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<th>(x,x+1/2,z [0,0,0])</th>
<th>(x+1/2,x,z [0,0,0])</th>
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<tr>
<td>4 b 2.mm1'</td>
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</table>

Symmetry of Special Projections

- Along \([0,0,1]\) p4mm1'
- Along \([1,0,0]\) p1m11'
- Along \([1,1,0]\) p1m11'

\(a^* = (a - b)/2\) \(b^* = (a + b)/2\)
Origin at 0,0,z

\(a^* = b/2\) \(b^* = c/2\)
Origin at x,0,0

\(a^* = (-a + b)/2\) \(b^* = c/2\)
Origin at x,x,0
**I4’c’m**

**4’c’m**

108.3.894

**Tetragonal**

**Origin** on 4’c’c

**Asymmetric unit**

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1; \quad y < \frac{1}{2} - x \]

**Symmetry Operations**

For \((0,0,0)\) + set

(1) 1
(1 | 0,0,0)

(2) 2 \(0,0,z\)
\((2_z | 0,0,0)\)

(3) \(4^+ \) \(0,0,z\)
\((4_z | 0,0,0)\)

(4) \(4^- \) \(0,0,z\)
\((4_z^{-1} | 0,0,0)\)

(5) \(a' \) \((1/2,0,0)\) \(x,1/4,z\)
\((m_y | 1/2,1/2,0)\)

(6) \(b' \) \((0,1/2,0)\) \(1/4,y,z\)
\((m_x | 1/2,1/2,0)\)

(7) \(m \) \(x+1/2,x,z\)
\((m_x | 1/2,1/2,0)\)

(8) \(g \) \((1/2,1/2,0)\) \(x,x,z\)
\((m_{xy} | 1/2,1/2,0)\)

For \((1/2,1/2,1/2)\) + set

(1) \(t \) \((1/2,1/2,1/2)\)
\((1 | 1/2,1/2,1/2)\)

(2) \(2 \) \((0,0,1/2)\) \(1/4,1/4,z\)
\((2_z | 1/2,1/2,1/2)\)

(3) \(4^+ \) \((0,0,1/2)\) \(0,1/2,z\)
\((4_z | 1/2,1/2,1/2)\)

(4) \(4^- \) \((0,0,1/2)\) \(1/2,0,z\)
\((4_z^{-1} | 1/2,1/2,1/2)\)

(5) \(c' \) \((0,0,1/2)\) \(x,0,z\)
\((m_y | 0,0,1/2)\)

(6) \(c' \) \((0,0,1/2)\) \(0,y,z\)
\((m_x | 0,0,1/2)\)

(7) \(c \) \((0,0,1/2)\) \(x,x,z\)
\((m_{xy} | 0,0,1/2)\)

(8) \(c \) \((0,0,1/2)\) \(x,x,z\)
\((m_{xy} | 0,0,1/2)\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

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<td>(2) x,x,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
</tbody>
</table>

8 c .m x,x+1/2,z [u,u,0] x+1/2,x+1/2,z [u,u,0] x+1/2,x,z [u,u,0]

4 b 2.mm 1/2,0,z [0,0,0] 0,1/2,z [0,0,0]

4 a 4'.. 0,0,z [0,0,0] 1/2,1/2,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm'  
\[a^* = (a - b)/2, \quad b^* = (a + b)/2\]

Origin at 0,0,z

Along [1,0,0] p1m1'  
\[a^* = b/2, \quad b^* = c/2\]

Origin at x,0,0

Along [1,1,0] p1m11'  
\[a^* = -(a + b)/2, \quad b^* = c/2\]

Origin at x,x,0
I4'c'm' 4'm'm' Tetragonal

108.4.895

Origin on 4'cc'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x \]

Symmetry Operations

For (0,0,0) + set

(1) \(1\) \(1\) (0,0,0) \(1\) (0,0,0)

(2) \(2\) 0,0,z \(2\) 0,0,0

(3) \(4^{+}\) 0,0,z \(4^{+}\) 0,0,0

(4) \(4^{-}\) 0,0,z \(4^{-}\) 0,0,0

(5) \(a\) (1/2,0,0) x,1/4,z \(m\) (1/2,1/2,0)

(6) \(b\) (0,1/2,0) 1/4,y,z \(m\) (1/2,1/2,0)

(7) \(m'\) \(1/2,1/2,0\) \(x+x,0,z\) \(m\) (1/2,1/2,0)

(8) \(g'\) (1/2,1/2,0) \(x,y,z\) \(m\) (1/2,1/2,0)

For (1/2,1/2,1/2) + set

(1) \(t\) (1/2,1/2,1/2) \(1\) (1/2,1/2,1/2)

(2) \(2\) (0,0,1/2) 1/4,1/4,z \(2\) (0,1/2,1/2)

(3) \(4^{+}\) (0,0,1/2) 0,1/2,z \(4^{+}\) (0,1/2,1/2)

(4) \(4^{-}\) (0,0,1/2) 1/2,0,z \(4^{-}\) (0,1/2,1/2)

(5) \(c\) (0,0,1/2) x,0,z \(m\) (0,0,1/2)

(6) \(c\) (0,0,1/2) 0,y,z \(m\) (0,0,1/2)

(7) \(c'\) (0,0,1/2) x,x,z \(m\) (0,0,1/2)

(8) \(c'\) (0,0,1/2) x,x,z \(m\) (0,0,1/2)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
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<tbody>
<tr>
<td>16 d 1 (1) x,y,z [u,v,w]</td>
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<td>(2) x,y,z [u,v,w]</td>
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<tr>
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<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
</tbody>
</table>

|8 c .m' x,x+1/2,z [u,u,w] |
|x,x+1/2,z [u,u,w] |
| x+1/2,x,z [u,u,w] |
| x+1/2,x,z [u,u,w] |

|4 b 2.m'm' 1/2,0,z [0,0,w] |
| 0,1/2,z [0,0,w] |

|2 a 4'.. 0,0,z [0,0,0] |
| 1/2,1/2,z [0,0,0] |

**Symmetry of Special Projections**

- **Along [0,0,1]**: p4'm'm
  - \(a^* = (a - b)/2\)
  - \(b^* = (a + b)/2\)
  - Origin at 0,0,z

- **Along [1,0,0]**: p1m'1
  - \(a^* = b/2\)
  - \(b^* = c/2\)
  - Origin at x,0,0

- **Along [1,1,0]**: p1m'1
  - \(a^* = -(a + b)/2\)
  - \(b^* = c/2\)
  - Origin at x,x,0
Tetragonal

### Origin on 4c'c'

### Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x \]

### Symmetry Operations

#### For \((0,0,0) +\) set

1. \(1\) \(0,0,0\)
2. \(2\) \(0,0,z\) \(2z\)
3. \(4^+\) \(0,0,z\) \(4z\)
4. \(4^-\) \(0,0,z\) \(4z^{-1}\)
5. \(a' (1/2,0,0)\) \(x,1/4,z\) \(m_{y1/2,1/2,0}'\)
6. \(b' (0,1/2,0)\) \(1/4,y,z\) \(m_{x1/2,1/2,0}'\)
7. \(m' x+1/2,\bar{x},z\) \(m_{xy1/2,1/2,0}'\)
8. \(g' (1/2,1/2,0)\) \(x,x,z\) \(m_{xy1/2,1/2,0}'\)

#### For \((1/2,1/2,1/2) +\) set

1. \(t (1/2,1/2,1/2)\)
2. \(2 (0,0,1/2)\) \(1/4,1/4,z\) \(2z\)
3. \(4^+ (0,0,1/2)\) \(0,1/2,z\) \(4z\)
4. \(4^- (0,0,1/2)\) \(1/2,0,z\) \(4z^{-1}\)
5. \(c' (0,0,1/2)\) \(x,0,z\) \(m_{y0,0,1/2}'\)
6. \(c' (0,0,1/2)\) \(y,z\) \(m_{x0,0,1/2}'\)
7. \(c' (0,0,1/2)\) \(x,x,z\) \(m_{xy0,0,1/2}'\)
8. \(c' (0,0,1/2)\) \(x,x,z\) \(m_{xy0,0,1/2}'\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(2) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
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<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td>8 c ..m' x,x+1/2,z [u,u,w]</td>
<td>x,x+1/2,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x,z [u,u,w]</td>
</tr>
<tr>
<td>4 b 2.m'm' 1/2,0,0, [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 a 4.. 0,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4m'm'</th>
<th>Along [1,0,0] p1m'1</th>
<th>Along [1,1,0] p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>a</strong> = (a - b)/2</td>
<td><strong>a</strong> = b/2</td>
<td><strong>a</strong> = -(a + b)/2</td>
</tr>
<tr>
<td><strong>b</strong> = (a + b)/2</td>
<td><strong>b</strong> = c/2</td>
<td><strong>b</strong> = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin on 4c'c'

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x\]

Symmetry Operations

For (0,0,0) + set

1. \(1\) (1) \(0,0,0\)
   \(1^*\) \(1/2,0,0\)

5. \(a\) \((1/2,0,0)\) \(x,1/4,z\)
   \((m_y|x/2,1/2,0)\)

(5) \(a\) \((1/2,0,0)\) \(x,1/4,z\)
   \((m_y|x/2,1/2,0)\)

6. \(b\) \((0,1/2,0)\) \(1/4,1/4,z\)
   \((m_x|x/2,1/2,0)\)

7. \(m\) \(x+1/2,x,z\)
   \((m_x|x/2,1/2,0)\)

8. \(g\) \((1/2,1/2,0)\) \(x,x,z\)
   \((m_x|x,1/2,1/2,0)\)

For \((1/2,1/2,1/2)' + set\)

1. \(t'\) \((1/2,1/2,1/2)'\)

2. \(t'\) \((0,0,1/2)\) \(1/4,1/4,z\)
   \((2_x|x/2,1/2,1/2)'\)

3. \(4^*\) \((0,0,1/2)\) \(0,1/2,z\)
   \((4_x|0,0,1/2)'\)

4. \(4^*\) \((0,0,1/2)\) \(0,1/2,z\)
   \((4_x|0,0,1/2)'\)

5. \(c'\) \((0,0,1/2)'\) \(x,0,z\)
   \((m_y|0,0,1/2)'\)

6. \(c'\) \((0,0,1/2)'\) \(0,y,z\)
   \((m_x|0,0,1/2)'\)

7. \(c'\) \((0,0,1/2)'\) \(x,x,z\)
   \((m_y|0,0,1/2)'\)

8. \(c'\) \((0,0,1/2)'\) \(x,x,z\)
   \((m_y|0,0,1/2)'\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>8</td>
<td>c .m</td>
<td>x,x+1/2,z [u,u,0] x+1/2,x [u,u,0] x+1/2,x [u,u,0] x+1/2,x [u,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>b 2.mm</td>
<td>1/2,0,z [0,0,0] 0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 4..</td>
<td>0,0,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p_4mm
  \( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)
- Origin at 0,0,z

- Along [1,0,0] p_2a1m
  \( a^* = b/2 \) \( b^* = c/2 \)
- Origin at x,1/4,0

- Along [1,1,0] p111
  \( a^* = -(a + b)/2 \) \( b^* = c/2 \)
- Origin at x,x,0
Tetragonal

**Origin on 4'cc'**

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \((1) 1 \quad (1|0,0,0)\)
2. \((2) 2 \quad 0,0,z \quad (2|0,0,0)\)
3. \((3) 4^{+} \quad 0,0,z \quad (4|0,0,0)\)'
4. \((4) 4^{-} \quad 0,0,z \quad (4|0,0,0)'\)

5. \((5) a'(1/2,0,0) \quad x,1/4,z \quad (m_{x}|1/2,1/2,0)'\)
6. \((6) b'(0,1/2,0) \quad 1/4,y,z \quad (m_{z}|1/2,1/2,0)'\)
7. \((7) m \quad x+1/2,x,z \quad (m_{x}|1/2,1/2,0)\)
8. \((8) g \quad (1/2,1/2,0) \quad x,x,z \quad (m_{z}|1/2,1/2,0)\)

For \((1/2,1/2,1/2)' + \) set

1. \((1) t' \quad (1/2,1/2,1/2) \quad (1|1/2,1/2,1/2)'\)
2. \((2) 2' \quad (0,0,1/2) \quad 1/4,1/4,z \quad (2|1/2,1/2,1/2)'\)
3. \((3) 4^{+} \quad (0,0,1/2) \quad 0,1/2,z \quad (4|1/2,1/2,1/2)'\)
4. \((4) 4^{-} \quad (0,0,1/2) \quad 1/2,0,z \quad (4|1/2,1/2,1/2)'\)

5. \((5) c(0,0,1/2) \quad x,0,z \quad (m_{z}|0,0,1/2)\)
6. \((6) c(0,0,1/2) \quad 0,y,z \quad (m_{z}|0,0,1/2)\)
7. \((7) c'(0,0,1/2) \quad x,x,z \quad (m_{x}|0,0,1/2)'\)
8. \((8) c'(0,0,1/2) \quad x,x,z \quad (m_{x}|0,0,1/2)'\)
Generators selected

(1); t(1,0,0); t(0,1,0); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
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<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
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<tr>
<td>(2) x',y',z [u',v',w']</td>
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<tr>
<td>(3) y',x,z [v',u',w']</td>
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<td>(4) y,x,z [v,u,w]</td>
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<tr>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x',y'+1/2,z [u',v',w']</td>
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<tr>
<td>(8) y+1/2,x+1/2,z [v',u',w']</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p,4mm a* = (a - b)/2 b* = (a + b)/2 Origin at 0,1/2,z
Along [1,0,0] p1m'1 a* = b/2 b* = c/2 Origin at x,0,0
Along [1,1,0] p1m11' a* = (a + b)/2 b* = c/2 Origin at x,x,0

Symmetry of Special Projections

Along [0,0,1] p,4mm a* = (a - b)/2 b* = (a + b)/2 Origin at 0,1/2,z
Origin on $4\overline{c}c$

Asymmetric unit

$$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x$$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1

(2) 2 $ 0,0,z$

(3) $4^* \cdot 0,0,z$

(4) $4^- \cdot 0,0,z$

(5) a $(1/2,0,0)$ $x,1/4,z$

(6) b $(0,1/2,0)$ $1/4,y,z$

(7) $m' \cdot x+1/2, x,z$

(8) $g' (1/2,1/2,0)$ $x,x,z$

For $(1/2,1/2,1/2)' +$ set

(1) $t' (1/2,1/2,1/2)$

(2) $2' (0,0,1/2)$ $1/4,1/4,z$

(3) $4^* (0,0,1/2)$ $0,1/2,z$

(4) $4^- (0,0,1/2)$ $1/2,0,z$

(5) $c' (0,0,1/2) \cdot x,0,z$

(6) $c' (0,0,1/2) \cdot 0,y,z$

(7) $c (0,0,1/2) \cdot \bar{x},z$

(8) $c (0,0,1/2) \cdot x,z$

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**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

**Positions**

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<td>(2) x′,y,z [u′,v′,w′]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z [u′,v′,w′]</td>
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<td>(7) y′+1/2,x′+1/2,z [v′,u′,w′]</td>
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<tr>
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<td>c ′</td>
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<td>x′,x+1/2,z [u′,u′,w′]</td>
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<tr>
<td>4</td>
<td>b ′</td>
<td>0,1/2,z [0,0,w]</td>
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<tr>
<td>2</td>
<td>a ′</td>
<td>0,0,z [0,0,0]</td>
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<td>1/2,1/2,z [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] \( p_2 \cdot 4m′m′ \)

\[ \mathbf{a}^* = \mathbf{a} - \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{a} + \mathbf{b}/2 \]

Origin at 0,1/2,z

Along [1,0,0] \( p_{2\alpha} \cdot 1m1 \)

\[ \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]

Origin at x,1/4,0

Along [1,1,0] \( p_{2\alpha} \cdot 1m1 \)

\[ \mathbf{a}^* = -(\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]

Origin at x,x,0
Origin on 4cc

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2 - x \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(\mathbf{1}\)
   
   \[(1) \mathbf{1} \quad (1|0,0,0)\]

2. \(\mathbf{2}\)
   
   \[(2) \mathbf{2} \quad 0,0,z \quad (2z|0,0,0)\]

3. \(\mathbf{4}^+\)
   
   \[(3) \mathbf{4}^+ \quad 0,0,z \quad (4z|0,0,0)\]

4. \(\mathbf{4}^-\)
   
   \[(4) \mathbf{4}^- \quad 0,0,z \quad (4z^{-1}|0,0,0)\]

\[(5) \mathbf{a}' \quad (1/2,0,0) \quad x,1/4,z\]

\[(m_y|1/2,1/2,0)'\]

\[(6) \mathbf{b}' \quad (0,1/2,0) \quad 1/4,y,z\]

\[(m_x|1/2,1/2,0)'\]

\[(7) \mathbf{m}' \quad x+1/2,x,z\]

\[(m_x|1/2,1/2,0)'\]

\[(8) \mathbf{g}' \quad (1/2,1/2,0) \quad x,x,z\]

\[(m_{xy}|1/2,1/2,0)'\]

For \((1/2,1/2,1/2)' + \) set

1. \(\mathbf{1}'\)
   
   \[(1) \mathbf{1}' \quad (1/2,1/2,1/2)\]

\[(1|1/2,1/2,1/2)'\]

\[(5) \mathbf{c} \quad (0,0,1/2) \quad x,0,z\]

\[(m_y|0,0,1/2)\]

\[(6) \mathbf{c} \quad (0,0,1/2) \quad 0,y,z\]

\[(m_x|0,0,1/2)\]

\[(7) \mathbf{c} \quad (0,0,1/2) \quad x,x,z\]

\[(m_{xy}|0,0,1/2)\]

\[(8) \mathbf{c} \quad (0,0,1/2) \quad x,x,z\]

\[(m_{xy}|0,0,1/2)\]
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

---

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>d</td>
<td>1</td>
<td>(0,0,0) + (1/2,1/2,1/2)’ +</td>
</tr>
<tr>
<td>8</td>
<td>c</td>
<td>m'</td>
<td>x,x+1/2,z [u,u,w] x,x+1/2,z [u,u,w] x+1/2,x,z [u,u,w] x+1/2,x,z [u,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>m’ m’</td>
<td>1/2,0,z [0,0,w] 0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4</td>
<td>0,0,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_4m'</th>
<th>4m'm'</th>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
<th>Along [1,1,0]</th>
<th>p2v-1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>a* = b/2 b* = c/2</td>
<td>a* = (a + b)/2 b* = c/2</td>
<td>a* = (-a + b)/2 b* = c/2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0
Origin on 2mm on 2m1

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
2. $2 \quad 0,0,z$
   
   (2) $2 \quad 0,0,0$

3. $4^+ \quad (0,0,1/4) \quad -1/4,1/4,z$
   
   (4) $4^+ \quad (0,0,1/4) \quad 1/4,1/4,z$
   
   (4) $4^+ \quad (0,0,1/4) \quad 1/4,1/4,z$

5. $m \quad x,0,z$
   
   (m) $x,0,0,0$

6. $m \quad 0,y,z$
   
   (m) $0,0,0,0$

7. $d \quad (-1/4,1/4,1/4) \quad x+1/4,x,z$
   
   (d) $d \quad (1/4,1/4,1/4) \quad x-1/4,x,z$

8. $d \quad (1/4,1/4,1/4) \quad x,1/4,x,z$
   
   (d) $d \quad (1/4,1/4,1/4) \quad x,1/4,x,z$

For $(1/2,1,2,1/2) +$ set

1. $t \quad (1/2,1/2,1/2)$
   
   (1) $t \quad 1/2,1/2,1/2$

2. $2 \quad (0,0,1/2) \quad 1/4,1/4,z$
   
   (2) $2 \quad (0,0,1/2) \quad 1/2,1/2,1/2$

3. $4^+ \quad (0,0,3/4) \quad 1/4,1/4,z$
   
   (3) $4^+ \quad (0,0,3/4) \quad 1/2,0,3/4$

4. $4^+ \quad (0,0,3/4) \quad 1/4,-1/4,z$
   
   (4) $4^+ \quad (0,0,3/4) \quad 1/4,-1/4,z$

5. $n \quad (1/2,0,1/2) \quad x,1/4,z$
   
   (m) $x,1/2,1/2,1/2$

6. $n \quad (0,1/2,1/2) \quad 1/4,y,z$
   
   (m) $0,1/2,1/2,1/2$

7. $d \quad (1/4,-1/4,3/4) \quad x+1/4,x,z$
   
   (d) $d \quad (1/4,-1/4,3/4) \quad x+1/4,x,z$

8. $d \quad (1/4,1/4,3/4) \quad x+1/4,x,z$
   
   (d) $d \quad (1/4,1/4,3/4) \quad x+1/4,x,z$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>c</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) y,x+1/2,z+1/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(8) y,x+1/2,z+1/4 [v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm     Along [1,0,0] c1m11'     Along [1,1,0] c_p1m1
a* = (a - b)/2  b* = (a + b)/2  a* = b  b* = c  a* = (-a + b)/2  b* = c/2
Origin at 1/4,1/4,z     Origin at x,0,0     Origin at x,x,0
Origin on 2mm1' on 2m11'

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For \((0,0,0) + \text{set}\):

1. \(1\)
2. \(2\) 0,0,z  
   \((2_z)0,0,0\)  
3. \(4^+ (0,0,1/4) -1/4,1/4,z \)  
   \((4_z)0,1/2,1/4\)  
4. \(4^- (0,0,1/4) 1/4,1/4,z \)  
   \((4_z^{-1})0,1/2,1/4\)

For \((1/2,1/2,1/2) + \text{set}\):

1. \(t\) \((1/2,1/2,1/2)\)
2. \(2\) \((0,0,1/4) 1/4,1/4,z \)  
   \((2_z)1/2,1/2,1/2\)  
3. \(4^+ (0,0,3/4) 1/4,1/4,z \)  
   \((4_z)1/2,0,3/4\)  
4. \(4^- (0,0,3/4) 1/4,-1/4,z \)  
   \((4_z^{-1})1/2,0,3/4\)

109.2.902 - 1 - 1797
Continued

For (0,0,0) + set

(1) 1' (0,0,0)'
   (2) 2' 0,0,z
        (2_1' 0,0,0)'
   (3) 4* (0,0,1/4) -1/4,1/4,z
        (4_2' 0,1/2,1/4)'
(5) m' x,0,z
    (m_x 0,0,0)'
(6) m' 0,y,z
    (m_y 0,0,0)'
(7) d' (-1/4,1/4,1/4) x+1/4,x,z
     (m_{xy} 0,1/2,1/4)'
(8) d' (1/4,1/4,1/4) x-1/4,x,z
    (m_{xy} 0,1/2,1/4)'

For (1/2,1/2,1/2) + set

(1) t' (1/2,1/2,1/2) (1/2,1/2,1/2)'
   (2) 2' (0,0,1/2) 1/4,1/4,z
        (2_2' 1/2,1/2,1/2)'
   (3) 4* (0,0,3/4) 1/4,1/4,z
        (4_2' 1/2,0,3/4)'
(5) n' (1/2,0,1/2) x,1/4,z
    (m_x 1/2,1/2,1/2)'
(6) n' (0,1/2,1/2) 1/4,y,z
    (m_y 1/2,1/2,1/2)'
(7) d' (1/4,-1/4,3/4) x+1/4,x,z
     (m_{xy} 1/2,0,3/4)'
(8) d' (1/4,1/4,3/4) x+1/4,x,z
    (m_{xy} 1/2,0,3/4)'

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Mult.</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 16    | x,y,z [0,0,0] | (0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)'
|       | x,y,z [0,0,0] | (1) x,y,z [0,0,0] |
|       | x,y,z [0,0,0] | (2) x,y,z [0,0,0] |
|       | x,y,z [0,0,0] | (3) y,x+1/2,z+1/4 [0,0,0] |
|       | x,y,z [0,0,0] | (4) y,x+1/2,z+1/4 [0,0,0] |
|       | x,y,z [0,0,0] | (5) x,y,z [0,0,0] |
|       | x,y,z [0,0,0] | (6) x,y,z [0,0,0] |
|       | x,y,z [0,0,0] | (7) y,x+1/2,z+1/4 [0,0,0] |
|       | y,x+1/2,z+1/4 [0,0,0] | (8) y,x+1/2,z+1/4 [0,0,0] |
| 8     | 0,y,z [0,0,0] | 0,y,z [0,0,0] |
|       | 0,y,z [0,0,0] | (0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)'
|       | 0,y,z [0,0,0] | (2) x,y,z [0,0,0] |
|       | 0,y,z [0,0,0] | (3) y,x+1/2,z+1/4 [0,0,0] |
|       | 0,y,z [0,0,0] | (4) y,x+1/2,z+1/4 [0,0,0] |
|       | 0,y,z [0,0,0] | (5) x,y,z [0,0,0] |
|       | 0,y,z [0,0,0] | (6) x,y,z [0,0,0] |
|       | 0,y,z [0,0,0] | (7) y,x+1/2,z+1/4 [0,0,0] |
|       | 0,y,z [0,0,0] | (8) y,x+1/2,z+1/4 [0,0,0] |
| 4     | 0,0,z [0,0,0] | 0,1/2,z+1/4 [0,0,0] |
|       | 0,0,z [0,0,0] | (0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)'

Symmetry of Special Projections

Along [0,0,1] p4gm1'

a* = (a - b)/2
b* = (a + b)/2

Origin at 1/4,1/4,z

Along [1,0,0] c1m11'

a* = b
b* = c

Origin at x,0,0

Along [1,1,0] c1m11'

a* = (-a + b)/2
b* = c/2

Origin at x,x,0
**Origin** on 2m'm' on 2m'1

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \((1)\) 1
   - \((1') 0,0,0\)
2. \((2)\) \(0,0,z\)
   - \((2') 0,0,0\)
3. \((3)\) \(4^+ (0,0,1/4) -1/4,1/4,z\)
   - \((3') 4^+ (0,0,1/4) 1/4,1/4,z\)
4. \((4)\) \((0,0,1/4) 0,1/2,1/4'\)
   - \((4') 0,1/2,1/4'\)

For \((1/2,1/2,1/2) + \) set

1. \((1)\) \(t(1/2,1/2,1/2)\)
   - \((1') 1/2,1/2,1/2\)
2. \((2)\) \((0,0,1/2) 1/4,1/4,z\)
   - \((2') 1/2,1/2,1/2\)
3. \((3)\) \(4^+ (0,0,3/4) 1/4,1/4,z\)
   - \((3') 4^+ (0,0,3/4) 1/2,0,3/4'\)
4. \((4)\) \((0,0,3/4) 0,1/2,1/4'\)
   - \((4') 0,1/2,1/4'\)

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**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**  
Multiplicities, Wyckoff letter, Site Symmetry, Coordinates.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>c</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p4'gm'  
  \(a^* = (a - b)/2\)  \(b^* = (a + b)/2\)  
  Origin at 1/4,1/4,z

- Along [1,0,0] c1m'1  
  \(a^* = b\)  \(b^* = c\)  
  Origin at x,0,0

- Along [1,1,0] c\(_p\)1m'1  
  \(a^* = (-a + b)/2\)  \(b^* = c/2\)  
  Origin at x,x,0
Origin on 2mm on 2m1

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2} \]

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\) \(0,0,0\)
2. \(2\) \(0,0,z\) \(2z,0,0,0\)
3. \(4'\) \(0,0,1/4\) \(-1/4,1/4,z\) \(4z,0,1/2,1/4\)
4. \(4\) \(0,0,1/4\) \(1/4,1/4,z\) \(4z^{-1},0,1/2,1/4\)

(5) \(m\) \(x,0,z\) \(m_x,0,0,0\)
(6) \(m\) \(0,y,z\) \(m_y,0,0,0\)
(7) \(d'\) \((-1/4,1/4,1/4)\) \(x+1/4,x,z\) \(m_x,0,1/2,1/4\)
(8) \(d'\) \((1/4,1/4,1/4)\) \(x-1/4,x,z\) \(m_x,0,1/2,1/4\)

For \((1/2,1/2,1/2)\) + set

1. \(t\) \((1/2,1/2,1/2)\)
2. \(2\) \((0,0,1/2)\) \(1/4,1/4,z\) \(2z,1/2,1/2,1/2\)
3. \(4'\) \((0,0,3/4)\) \(1/4,1/4,z\) \(4z,1/2,0,3/4\)
4. \(4\) \((0,0,3/4)\) \(1/4,-1/4,z\) \(4z^{-1},1/2,0,3/4\)

(5) \(n\) \((1/2,0,1/2)\) \(x,1/4,z\) \(m_x,1/2,1/2,1/2\)
(6) \(n\) \((0,1/2,1/2)\) \(1/4,y,z\) \(m_y,1/2,1/2,1/2\)
(7) \(d'\) \((1/4,-1/4,3/4)\) \(x+1/4,x,z\) \(m_x,1/2,0,3/4\)
(8) \(d'\) \((1/4,1/4,3/4)\) \(x+1/4,x,z\) \(m_x,1/2,0,3/4\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

\[(0,0,0) + (1/2,1/2,1/2) + \]

16 c 1 (1) x,y,z [u,v,w] (2) \( \bar{x},y,z [\bar{u},\bar{v},\bar{w}] \)

(3) \( y,x+1/2,z+1/4 [v,\bar{u},\bar{w}] \) (4) y,\( x+1/2,z+1/4 [\bar{v},u,\bar{w}] \)

(5) x,\( y,z [u,v,w] \) (6) \( x,y,z [u,\bar{v},\bar{w}] \)

(7) \( y,x+1/2,z+1/4 [\bar{v},u,w] \) (8) \( y,x+1/2,z+1/4 [v,u,w] \)

8 b .m. 0,y,z [u,0,0] 0,y,1/2,z+1/4 [0,u,0]

4 a 2mm. 0,0,z [0,0,0] 0,1/2,z+1/4 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along</th>
<th>p4'g'm</th>
<th>c1m11'</th>
<th>c1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>( a^* = (a - b)/2 ) ( b^* = (a + b)/2 )</td>
<td>( a^* = b ) ( b^* = c )</td>
<td>( a^* = (a + b)/2 ) ( b^* = c/2 )</td>
</tr>
<tr>
<td>Origin at 1/4,1/4,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
I4, m’d’

4m’m’

109.5.905

Tetragonal

Origin on 2m’m’ on 2m’1

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) 0,0,0

(3) 4’ (0,0,1/4) -1/4,1/4,z
(4,z,0,1/2,1/4)

(4) 4’ (0,0,1/4) 1/4,1/4,z
(4,z,1/2,1/4)

(5) m’ x,0,z
(5 m’ x,0,0,0)

(6) m’ 0,y,z
(6 m’ 0,0,0)

(7) d’ (-1/4,1/4,1/4) x+1/4,x,z
(m,0,1/2,1/4)

(8) d’ (1/4,1/4,1/4) x+1/4,x,z
(m,0,1/2,1/4)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2,1/2)
(1/2,1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2) 1/2,1/2,1/2,1/2

(3) 4’ (0,0,3/4) 1/4,1/4,z
(4,z,1/2,0,3/4)

(4) 4’ (0,0,3/4) 1/4,-1/4,z
(4,z,1/2,0,3/4)

(5) n’ (1/2,0,1/2) x,1/4,z
(5 m,1/2,1/2,1/2)

(6) n’ (0,1/2,1/2) 1/4,y,z
(6 m,1/2,1/2,1/2)

(7) d’ (1/4,-1/4,3/4) x+1/4,x,z
(m,1/2,0,3/4)

(8) d’ (1/4,1/4,3/4) x+1/4,x,z
(m,1/2,0,3/4)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 c</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
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<tr>
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</tr>
</tbody>
</table>

**Coordinates**

(0,0,0) + (1/2,1/2,1/2) +

---

**Symmetry of Special Projections**

Along [0,0,1] p4g'm'

<table>
<thead>
<tr>
<th>a* = (a - b)/2</th>
<th>b* = (a + b)/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at 1/4,1/4,z</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>

Along [1,0,0] c1m'1

<table>
<thead>
<tr>
<th>a* = b</th>
<th>b* = c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

Along [1,1,0] c1m'1

<table>
<thead>
<tr>
<th>a* = -(a + b)/2</th>
<th>b* = c/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
**Origin** on 2c1

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

For \((0,0,0) + \text{ set}\):

1. \((0,0,0)\)
2. \(0,0,z\)
3. \(0,1/2,1/4\)
4. \(0,1/4,1/4,1/4\)
5. \(0,1/2,0\)
6. \(0,1/2,1/2\)
7. \(0,1/4,1/4\)
8. \(0,1/4,1/4,1/4\)
9. \(0,1/2,0\)
10. \(0,1/2,1/2\)

For \((1/2,1/2,1/2) + \text{ set}\):

1. \((1/2,1/2,1/2)\)
2. \(1/4,1/4,1/4\)
3. \(1/4,1/4,1/4\)
4. \(1/2,0,1/2\)
5. \(1/2,1/2,0\)
6. \(1/2,1/2,1/2\)
7. \(1/4,1/4,1/4\)
8. \(1/4,1/4,1/4\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Continued

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>b</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1/2,1/2,1/2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x+1/2,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) y,x+1/2,z+3/4 [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm
Along [1,0,0] p2b1m1
Along [1,1,0] c1m1

a* = (a - b)/2   b* = (a + b)/2
a* = b/2   b* = c/2
a* = (-a + b)/2   b* = c/2

Origin at 1/4,1/4,z
Origin at x,0,0
Origin at x,x,0
**Symmetry Operations**

**Origin** on 2c11'

**Asymmetric unit**  
$0 \leq x < 1/2$;  $0 \leq y < 1/2$;  $0 \leq z < 1/4$

### For $(0,0,0)$ + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td></td>
</tr>
<tr>
<td>(1) 0,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) 2</td>
<td>0,0,z</td>
</tr>
<tr>
<td>(2) 0,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3) 4⁺</td>
<td>(0,0,1/4) -1/4,1/4,z</td>
</tr>
<tr>
<td>(4) 4⁺</td>
<td>(0,0,1/4) 1/4,1/4,z</td>
</tr>
</tbody>
</table>

### For $(1/2,1/2,1/2)$ + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t</td>
<td>(1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(1) 1/2,1/2,1/2</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) 2</td>
<td>(0,0,1/2) 1/4,1/4,z</td>
</tr>
<tr>
<td>(2) 1/2,1/2,1/2</td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
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</tr>
</thead>
<tbody>
<tr>
<td>(3) 4⁺</td>
<td>(0,0,3/4) 1/4,1/4,z</td>
</tr>
<tr>
<td>(4) 4⁺</td>
<td>(0,0,3/4) 1/4,-1/4,z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5) a</td>
<td>(1/2,0,0) x,1/4,z</td>
</tr>
<tr>
<td>(5) 1/2,1/2,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(6) b</td>
<td>(0,1/2,0) 1/4,y,z</td>
</tr>
<tr>
<td>(6) 1/2,1/2,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
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<tbody>
<tr>
<td>(7) d</td>
<td>(1/4,-1/4,1/4) x+1/4,x,z</td>
</tr>
<tr>
<td>(8) d</td>
<td>(1/4,1/4,1/4) x+1/4,x,z</td>
</tr>
</tbody>
</table>

### For $(0,0,1/4)$ + set

<table>
<thead>
<tr>
<th>Operation</th>
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<tbody>
<tr>
<td>(1) 1</td>
<td></td>
</tr>
<tr>
<td>(1) 0,0,1/4</td>
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<tr>
<td>(2) 2</td>
<td>0,0,z</td>
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<td>(2) 0,0,0</td>
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<td>(3) 4⁺</td>
<td>(0,0,1/4) -1/4,1/4,z</td>
</tr>
<tr>
<td>(4) 4⁺</td>
<td>(0,0,1/4) 1/4,1/4,z</td>
</tr>
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### For $(1/2,0,1/2)$ + set

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<tr>
<td>(1) t</td>
<td>(1/2,0,1/2)</td>
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<tr>
<td>(1) 1/2,0,1/2</td>
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<td>(5) a</td>
<td>(1/2,1/2,0) x,1/4,z</td>
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<td>(0,1/2,0) 1/4,y,z</td>
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### For $(1/2,1/2,0)$ + set

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<td>(1) t</td>
<td>(1/2,1/2,0)</td>
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<td>(1) 1/2,1/2,0</td>
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</tbody>
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<td>(2) 2</td>
<td>(0,0,1/2) 1/4,1/4,z</td>
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<td>(2) 1/2,1/2,0</td>
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</tr>
</tbody>
</table>
Continued

For (0,0,0)'+ set

(1) 1' 0,0,0' (2) 2' 0,0,z (3) 4' (0,0,1/4) 1/4,1/4,z (4) 4' (0,0,1/4) 1/4,1/4,z
   (1) 0,0,0' (2) 0,0,0' (3) 0,0,1/4 (4) 0,0,1/4

(5) c' (0,0,1/2) x,0,z (m|0,0,1/2)' (6) c' (0,0,1/2) 0,y,z (7) d' (-1/4,1/4,3/4) x+1/4,x,z
   (m|0,0,1/2)' (8) d' (1/4,1/4,3/4) x-1/4,x,z (m|0,0,1/2) + (1/2,1/2,1/2) +
   (m|0,0,1/2) (m|1/2,1/2,1/2) + (m|1/2,1/2,1/2)'

For (1/2,1/2,1/2)'+ set

(1) t' (1/2,1/2,1/2) (2) 2' (0,0,1/2) 1/4,1/4,z (3) 4' (0,0,3/4) 1/4,1/4,z (4) 4' (0,0,3/4) 1/4,-1/4,z
   (1) 1/2,1/2,1/2' (2) 1/2,1/2,1/2' (3) 1/2,0,3/4 (4) 1/2,0,3/4

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

Multiplicity
Wyckoff letter
Site Symmetry

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)'+</td>
<td></td>
</tr>
<tr>
<td>16 b 11'</td>
<td>(1) x,y,z [0,0,0] (2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x+1/2,z+1/4 [0,0,0] (4) y,x+1/2,z+1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [0,0,0] (6) x,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x+1/2,z+3/4 [0,0,0] (8) y,x+1/2,z+3/4 [0,0,0]</td>
</tr>
<tr>
<td>8 a 2..1'</td>
<td>0,0,z [0,0,0] 0,1/2,z+1/4 [0,0,0] 0,0,z+1/2 [0,0,0] 0,1/2,z+3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1' Along [1,0,0] p1m11' Along [1,1,0] c1m11'
\[
a^* = (a - b)/2 \quad b^* = (a + b)/2
\]
Origin at 1/4,1/4,z \[
a^* = b/2 \quad b^* = c/2
\]
Origin at x,0,0 \[
a^* = (-a + b)/2 \quad b^* = c/2
\]
Origin at x,x,0
I4₁' c'd

110.3.908

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1) |0,0,0|

(2) t (0,0,1/2) 0,0,z
   (2) |0,0,1/2|

(3) 4⁺ (0,0,1/4) -1/4,1/4,z
   (3) |0,1/2,1/4|

(4) 4⁻ (0,0,1/4) 1/4,1/4,z
   (4) |1/2,1/4|

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) 1/4,1/4,z
   (1) |1/2,1/2,1/2|

(2) 2 (0,0,1/2) 1/4,1/4,z
   (2) |1/2,1/2,1/2|

(3) 4⁺ (0,0,3/4) 1/4,1/4,z
   (3) |1/2,0,3/4|

(4) 4⁻ (0,0,3/4) 1/4,-1/4,z
   (4) |1/2,0,3/4|

(5) a' (1/2,0,0) x,1/4,z
   (5) |1/2,1/2,0|

(6) b' (0,1/2,0) 1/4,y,z
   (6) |1/2,1/2,0|

(7) d (1/4,-1/4,1/4) x+1/4,z
   (7) |1/2,0,1/4|

(8) d (1/4,1/4,1/4) x+1/4,z
   (8) |1/2,0,1/4|
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16</td>
<td>b 1</td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(2) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(3) y,x+1/2,z+1/4</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(4) y,x+1/2,z+1/4</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(5) x,y,z+1/2</td>
<td>[u,v,w]</td>
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<tr>
<td>(6) x,y,z+1/2</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(7) y,x+1/2,z+3/4</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(8) y,x+1/2,z+3/4</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>a 2..</td>
</tr>
<tr>
<td>0,0,z</td>
<td>[0,0,w]</td>
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<tr>
<td>0,1/2,z+1/4</td>
<td>[0,0,w]</td>
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<tr>
<td>0,0,z+1/2</td>
<td>[0,0,w]</td>
</tr>
<tr>
<td>0,1/2,z+3/4</td>
<td>[0,0,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4'gm'  
Along [1,0,0] p1m'1  
Along [1,1,0] c1m'1

\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]

Origin at 1/4,1/4,z  
Origin at x,0,0  
Origin at x,x,0
Origin on 2c1

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1| 0,0,0)

(2) 2 0,0,z
(2z| 0,0,0)

(3) 4' (0,0,1/4) -1/4,1/4,z
(4z| 0,1/2,1/4')

(4) 4' (0,0,1/4) 1/4,1/4,z
(4z| 0,1/2,1/4')

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1| 1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z
(2z| 1/2,1/2,1/2)

(3) 4' (0,0,3/4) 1/4,1/4,z
(4z| 1/2,0,3/4')

(4) 4' (0,0,3/4) 1/4,-1/4,z
(4z| 1/2,0,3/4')

For (1/2,1,2,1/2) + set

(5) a (1/2,0,0) x,1/4,z
(my| 1/2,1,2,0)

(6) b (0,1/2,0) 1/4,y,z
(mx| 1/2,1,2,0)

(7) d' (1/4,-1/4,1/4) x+1/4,z
(mx| 1/2,0,1/4')

(8) d' (1/4,1/4,1/4) x+1/4,z
(mx| 1/2,0,1/4')
Continued

110.4.909

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 b 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [v,u,w]</td>
<td>(6) x,y,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x+1/2,z+3/4 [v,u,w]</td>
<td>(8) y,x+1/2,z+3/4 [v,u,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p4'g'm</td>
</tr>
<tr>
<td>a* = (a - b)/2  b* = (a + b)/2</td>
</tr>
<tr>
<td>Origin at 1/4,1/4,z</td>
</tr>
</tbody>
</table>

| Along [1,0,0] p2b*1m'1 |
| a* = b/2  b* = c/2 |
| Origin at x,0,0 |

| Along [1,1,0] c1m'1 |
| a* = (-a + b)/2  b* = c/2 |
| Origin at x,x,0 |

**Symmetry of Special Projections**

| Along [0,1,0] p4'g'm |
| a* = (a - b)/2  b* = (a + b)/2 |
| Origin at 1/4,1/4,z |

| Along [1,0,0] p2b*1m'1 |
| a* = b/2  b* = c/2 |
| Origin at x,0,0 |

| Along [1,1,0] c1m'1 |
| a* = (-a + b)/2  b* = c/2 |
| Origin at x,x,0 |
Origin on 2c'1

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4} \]

Symmetry Operations

For \((0,0,0) +\) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 4^+ \ (0,0,1/4) -1/4,1/4,z \\
(4) & \quad 4^- \ (0,0,1/4) 1/4,1/4,z
\end{align*}
\]

\[
\begin{align*}
(1^*) & \quad 0,0,0 \\
(2^*) & \quad 0,0,0 \\
(3^*) & \quad 4^+ \ * (0,0,1/4) -1/4,1/4,z \\
(4^*) & \quad 4^- \ * (0,0,1/4) 1/4,1/4,z
\end{align*}
\]

\[
\begin{align*}
(5) & \quad c' \ (0,0,1/2) \ x,0,z \\
(6) & \quad c' \ (0,0,1/2) \ 0,y,z \\
(7) & \quad d' \ * (-1/4,1/4,3/4) \ x+1/4,x,z \\
(8) & \quad d' \ (1/4,1/4,3/4) \ x-1/4,x,z
\end{align*}
\]

\[
\begin{align*}
(5^*) & \quad m_y \ (0,0,1/2)' \\
(6^*) & \quad m_y \ (0,0,1/2)' \\
(7^*) & \quad m_y \ (0,1/2,3/4)' \\
(8^*) & \quad m_y \ (0,1/2,3/4)'
\end{align*}
\]

For \((1/2,1/2,1/2) +\) set

\[
\begin{align*}
(1) & \quad t \ (1/2,1/2,1/2) \\
(2) & \quad 2 \ (0,0,1/2) \ 1/4,1/4,z \\
(3) & \quad 4^+ \ * (0,0,3/4) 1/4,1/4,z \\
(4) & \quad 4^- \ * (0,0,3/4) 1/4,-1/4,z
\end{align*}
\]

\[
\begin{align*}
(1^*) & \quad 1/2,1/2,1/2 \\
(2^*) & \quad 1/2,1/2,1/2 \\
(3^*) & \quad 4^+ \ * (0,0,3/4) 1/4,1/4,z \\
(4^*) & \quad 4^- \ * (0,0,3/4) 1/4,-1/4,z
\end{align*}
\]

\[
\begin{align*}
(5) & \quad a' \ (1/2,0,0) \ x,1/4,z \\
(6) & \quad b' \ (0,1/2,0) \ 1/4,y,z \\
(7) & \quad d' \ * (1/4,-1/4,1/4) \ x+1/4,x,z \\
(8) & \quad d' \ (1/4,1/4,1/4) \ x+1/4,x,z
\end{align*}
\]

\[
\begin{align*}
(5^*) & \quad m_y \ (1/2,1/2,0)' \\
(6^*) & \quad m_y \ (1/2,1/2,0)' \\
(7^*) & \quad m_y \ (1/2,0,1/4)' \\
(8^*) & \quad m_y \ (1/2,0,1/4)'
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<th>Site Symmetry</th>
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<tr>
<td>16</td>
<td>b</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x+1/2,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) y,x+1/2,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>a</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,z+1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,z+3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm'

\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]

Origin at 1/4,1/4,z

Along [1,0,0] p1m'1

\[ a^* = b/2 \quad b^* = c/2 \]

Origin at x,0,0

Along [1,1,0] c1m'1

\[ a^* = -(a + b)/2 \quad b^* = c/2 \]

Origin at x,x,0
Origin on $\bar{4}2m$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

1. $1$
   
2. $2 \cdot 0,0,z$
   
3. $\bar{4} \cdot 0,0,0$

4. $\bar{4} \cdot 0,0,0$

5. $2 \cdot 0,y,0$

6. $2 \cdot x,0,0$

7. $m \cdot x,x,z$

8. $m \cdot x,x,z$

$P\bar{4}2m$

$\bar{4}2m$

Tetragonal
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions  
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>8</td>
<td>o</td>
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</tr>
<tr>
<td>4</td>
<td>n</td>
<td>..m</td>
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<tr>
<td>4</td>
<td>m</td>
<td>2..</td>
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<tr>
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<td>.2</td>
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<td>2</td>
<td>e</td>
<td>222</td>
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<tr>
<td>1</td>
<td>d</td>
<td>42m</td>
</tr>
<tr>
<td>1</td>
<td>c</td>
<td>42m</td>
</tr>
<tr>
<td>1</td>
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<td>42m</td>
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<tr>
<td>1</td>
<td>a</td>
<td>42m</td>
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Coordinates

<table>
<thead>
<tr>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) x,y,z [v,u,w]</th>
<th>(4) x,y,z [v,u,w]</th>
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</thead>
<tbody>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(7) x,y,z [v,u,w]</td>
<td>(8) x,y,z [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  
p4mm'  
a* = a  
b* = b  
Origin at 0,0,z

Along [1,0,0]  
p2m'm'  
a* = b  
b* = c  
Origin at x,0,0

Along [1,1,0]  
p1m11'  
a* = -(a + b)/2  
b* = c  
Origin at x,x,0
Origin on $\overline{4}2m1'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

For 1 + set

1. $1$
   \((1|0,0,0)\)
   \((1|0,0,0)\)

2. $2$ \(0,0,z\)
   \((2_z|0,0,0)\)

3. $\overline{4}^+ \quad 0,0,z; 0,0,0$
   \((4_z|0,0,0)\)

4. $\overline{4}^- \quad 0,0,z; 0,0,0$
   \((4_z^{-1}|0,0,0)\)

For 1' + set

1'. $1'$
   \((1|0,0,0)'\)

2'. $2' \quad 0,0,z$
   \((2_z|0,0,0)'\)

3'. $\overline{4}^+ ' \quad 0,0,z; 0,0,0$
   \((4_z|0,0,0)'\)

4'. $\overline{4}^- ' \quad 0,0,z; 0,0,0$
   \((4_z^{-1}|0,0,0)'\)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

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<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
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<td>( \cdot )</td>
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<table>
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<th>Coordinates</th>
<th>1+</th>
<th>( \cdot ) 1' +</th>
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<td>(8)</td>
<td>y,x,z [0,0,0]</td>
</tr>
<tr>
<td>( 1/2,0,1/2 [0,0,0] )</td>
<td>(4)</td>
<td>( y,x,z [0,0,0] )</td>
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<tr>
<td>( 1/2,0,z [0,0,0] )</td>
<td>(6)</td>
<td>( y,x,z [0,0,0] )</td>
</tr>
<tr>
<td>( 0,1/2,z [0,0,0] )</td>
<td>(7)</td>
<td>( y,x,z [0,0,0] )</td>
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<tr>
<td>( 0,0,1/2 [0,0,0] )</td>
<td>(1)</td>
<td>( y,x,z [0,0,0] )</td>
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<td>( 0,0,0 [0,0,0] )</td>
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<td>(9)</td>
<td>( y,x,z [0,0,0] )</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along ([0,0,1])</th>
<th>p4mm1'</th>
<th>Along ([1,0,0])</th>
<th>p2mm1'</th>
<th>Along ([1,1,0])</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a )</td>
<td></td>
<td>( a^* = a )</td>
<td></td>
<td>( a^* = (-a+b)/2 )</td>
<td></td>
</tr>
<tr>
<td>( b^* = b )</td>
<td></td>
<td>( b^* = c )</td>
<td></td>
<td>( b^* = c )</td>
<td></td>
</tr>
<tr>
<td>Origin at (0,0,z)</td>
<td></td>
<td>Origin at (x,0,0)</td>
<td></td>
<td>Origin at (x,x,0)</td>
<td></td>
</tr>
</tbody>
</table>
Origin on \( \bar{4}2'm \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \)

Symmetry Operations

1. \( 1 \)  
   \((1|0,0,0)\)

2. \( 2 \)  
   \((2|0,0,z)\)  
   \((2_z|0,0,0)\)

3. \( 4' \)  
   \((4|0,0,z)\)  
   \((4_z|0,0,0)\)

4. \( 4' \)  
   \((4|0,0,z)\)  
   \((4_z|0,0,0)\)

5. \( 2' \)  
   \((5,0,0)\)  
   \((2_y|0,0,0)\)

6. \( 2' \)  
   \((6|x,0,0)\)  
   \((2_x|0,0,0)\)

7. \( m \)  
   \((7|x,x,z)\)  
   \((m_{xy}|0,0,0)\)

8. \( m \)  
   \((8|x,x,z)\)  
   \((m_{xy}|0,0,0)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>8</th>
<th>o</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) x,z [v,u,w]</th>
<th>(4) y,x,z [v,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>m</td>
<td>x,z [u,u,0]</td>
<td>x,z [u,u,0]</td>
<td>x,z [u,u,0]</td>
<td>x,z [u,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>n</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>l</td>
<td>x,1/2,0 [0,v,w]</td>
<td>x,1/2,0 [0,v,w]</td>
<td>1/2,x,0 [v,0,w]</td>
<td>1/2,x,0 [v,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>k</td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
<td>0,x,1/2 [v,0,w]</td>
<td>0,x,1/2 [v,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>j</td>
<td>x,1/2,1/2 [0,v,w]</td>
<td>x,1/2,1/2 [0,v,w]</td>
<td>1/2,x,1/2 [v,0,w]</td>
<td>1/2,x,1/2 [v,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>i</td>
<td>0,0 [v,w]</td>
<td>0,0 [v,w]</td>
<td>0,0 [v,w]</td>
<td>0,0 [v,w]</td>
</tr>
<tr>
<td>2</td>
<td>h</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>g</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>f</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>d</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>c</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Coordinates

Symmetry of Special Projections

Along [0,0,1] p4m'm'  
\( a^* = a \)  \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p2'm'm'  
\( a^* = -c \)  \( b^* = b \)  
Origin at x,0,0

Along [1,1,0] p1m11'  
\( a^* = (a + b)/2 \)  \( b^* = c \)  
Origin at x,x,0
**Symmetry Operations**

1. \( 1 \)  
   1

2. \( 2 \)  
   \( 0,0,z \)  
   \( (2,0,0,0) \)

3. \( \bar{4} \)  
   \( 0,0,0; 0,0,0 \)  
   \( (\bar{4}_z|0,0,0) \)  
   \( (\bar{4}_z|0,0,0)' \)

4. \( \bar{m} \)  
   \( x,x,z \)  
   \( (m_x|0,0,0) \)  
   \( (m_x|0,0,0)' \)

5. \( 2 \)  
   \( 0,y,0 \)  
   \( (2,0,0,0) \)

6. \( 2 \)  
   \( x,0,0 \)  
   \( (2,0,0,0) \)

7. \( \bar{m} \)  
   \( x,x,z \)  
   \( (m_x|0,0,0) \)  
   \( (m_x|0,0,0)' \)

8. \( \bar{m} \)  
   \( x,x,z \)  
   \( (m_x|0,0,0) \)  
   \( (m_x|0,0,0)' \)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 o</td>
<td>1</td>
<td>x,y,z [u,v,w]</td>
<td>(1)</td>
</tr>
<tr>
<td>4 n</td>
<td>.m'</td>
<td>x,x,z [u,u,w]</td>
<td>(2)</td>
</tr>
<tr>
<td>4 m</td>
<td>2.</td>
<td>1/2,0,z [0,0,w]</td>
<td>(3)</td>
</tr>
<tr>
<td>4 l</td>
<td>.2.</td>
<td>x,1/2,0 [u,0,0]</td>
<td>(4)</td>
</tr>
<tr>
<td>4 k</td>
<td>.2.</td>
<td>x,0,1/2 [u,0,0]</td>
<td>(5)</td>
</tr>
<tr>
<td>4 j</td>
<td>.2.</td>
<td>x,1/2,1/2 [u,0,0]</td>
<td>(6)</td>
</tr>
<tr>
<td>4 i</td>
<td>.2.</td>
<td>x,0,0 [u,0,0]</td>
<td>(7)</td>
</tr>
<tr>
<td>2 h</td>
<td>2.m'm'</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>(8)</td>
</tr>
<tr>
<td>2 g</td>
<td>2.m'm'</td>
<td>0,0,z [0,0,w]</td>
<td>(9)</td>
</tr>
<tr>
<td>2 f</td>
<td>222.</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>(10)</td>
</tr>
<tr>
<td>2 e</td>
<td>222.</td>
<td>1/2,0,0 [0,0,0]</td>
<td>(11)</td>
</tr>
<tr>
<td>1 d</td>
<td>4'2m'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>(12)</td>
</tr>
<tr>
<td>1 c</td>
<td>4'2m'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>(13)</td>
</tr>
<tr>
<td>1 b</td>
<td>4'2m'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>(14)</td>
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<tr>
<td>1 a</td>
<td>4'2m'</td>
<td>0,0,0 [0,0,0]</td>
<td>(15)</td>
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</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 o</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 n</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>4 m</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 l</td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>4 k</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 j</td>
<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 i</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2 h</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2 g</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 f</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 e</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>1 d</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1 c</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>1 b</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>1 a</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm          Along [1,0,0] p2m'm'          Along [1,1,0] p1m'1  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  \[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]  \[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]  
Origin at 0,0,z             Origin at x,0,0             Origin at x,x,0  

111.4.914 - 2 - 1822
Origin on $\overline{4}2'm'$

Asymmetric unit  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y$

Symmetry Operations

1. $1$
2. $2$ 0,0,z
   (2z|0,0,0)
3. $\overline{4}'$ 0,0,z; 0,0,0
   ($\overline{4}_z|0,0,0$)
4. $\overline{4}'$ 0,0,z; 0,0,0
   ($\overline{4}_z|0,0,0$)
5. $2'$ 0,y,0
   (2y|0,0,0)'
6. $2'$ x,0,0
   (2x|0,0,0)'
7. $m'$ x,x,z
   (mxy|0,0,0)'
8. $m'$ x,x,z
   (mxy|0,0,0)'}
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Series</th>
<th>Multiplicity</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>n .m'</td>
<td>x,x,z [u,u,w]</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>m 2..</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>l .2'</td>
<td>x,1/2,0 [0,v,w]</td>
<td>x,1/2,0 [0,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>k .2'</td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>j .2'</td>
<td>x,1/2,1/2 [0,v,w]</td>
<td>x,1/2,1/2 [0,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>i .2'</td>
<td>x,0,0 [0,v,w]</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>h 2.m'm'</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>g 2.m'm'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>f 22'2'</td>
<td>1/2,0,1/2 [0,0,w]</td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>e 22'2'</td>
<td>1/2,0,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>d 42'm'</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>c 42'm'</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>b 42'm'</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>a 42'm'</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'mm'  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2'mm'  
\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at x,0,0

Along [1,1,0] p1m'1
\[ \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,0
Origin on \( \overline{4}2m \)

Asymmetric unit \( 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1; \quad x < y \)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad \overline{4}^+ \quad 0,0,z; \quad 0,0,0 \\
(4) & \quad \overline{4}^+ \quad 0,0,z; \quad 0,0,0 \\
(5) & \quad 2 \quad 0,y,0 \\
(6) & \quad 2 \quad x,0,0 \\
(7) & \quad m \quad x,x,z \\
(8) & \quad m \quad x,x,z
\end{align*}
\]

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(2) & \quad 2' \quad (0,0,1) \\
(3) & \quad \overline{4}'^- \quad 0,0,z; \quad 0,0,1/2 \\
(4) & \quad \overline{4}'^- \quad 0,0,z; \quad 0,0,1/2 \\
(5) & \quad 2' \quad 0,y,1/2 \\
(6) & \quad 2' \quad x,0,1/2 \\
(7) & \quad c' \quad (0,0,1) \quad x,x,z \\
(8) & \quad c' \quad (0,0,1) \quad x,x,z
\end{align*}
\]

111.6.916 - 1 - 1825
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{array}{cccc}
\text{Multiplicity} & \text{Wyckoff letter} & \text{Site Symmetry} & \text{Coordinates} \\
16 & o & 1 & (1) x,y,z [u,v,w] (2) \bar{x},y,\bar{z} [\bar{u},\bar{v},\bar{w}] (3) y,x,\bar{z} [v,u,0] (4) y,\bar{x},\bar{z} [v,u,0] \\
8 & n & .m & x,x,z [u,u,0] x,x,z [u,u,0] x,x,z [u,u,0] x,x,z [u,u,0] \\
8 & m & .2. & 0,1/2,0 [0,0,w] 1/2,0,\bar{z} [0,0,w] 0,1/2,\bar{z} [0,0,w] 0,1/2,\bar{z} [0,0,w] \\
8 & l & .2. & x,1/2,0 [u,0,0] x,1/2,0 [u,0,0] 1/2,x,0 [u,0,0] 1/2,x,0 [u,0,0] \\
8 & k & .2'. & x,0,1/2 [0,v,w] \bar{x},0,1/2 [0,\bar{v},\bar{w}] 0,x,1/2 [v,0,w] 0,x,1/2 [v,0,w] \\
8 & j & .2'. & x,1/2,1/2 [0,v,w] \bar{x},1/2,1/2 [0,\bar{v},\bar{w}] 1/2,x,1/2 [v,0,w] 1/2,x,1/2 [v,0,w] \\
8 & i & .2. & x,0,0 [u,0,0] \bar{x},0,0 [\bar{u},\bar{0},\bar{0}] 0,\bar{x},0 [u,0,0] 0,\bar{x},0 [u,0,0] \\
4 & h & 2mm & 1/2,1/2,0 [0,0,0] 1/2,1/2,\bar{z} [0,0,0] 1/2,1/2,\bar{z} [0,0,0] \\
4 & g & 2mm & 0,0,z [0,0,0] 0,0,z [0,0,0] 0,0,z [0,0,0] 0,0,z [0,0,0] \\
4 & f & 22'2' & 1/2,0,1/2 [0,0,w] 0,1/2,1/2 [0,0,w] 0,1/2,1/2 [0,0,w] 0,1/2,1/2 [0,0,w] \\
4 & e & 222. & 1/2,0,0 [0,0,0] 0,1/2,0 [0,0,0] 0,1/2,0 [0,0,0] 0,1/2,0 [0,0,0] \\
2 & d & 42m & 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] \\
2 & c & 4'2m & 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0] \\
2 & b & 4'2m & 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] \\
2 & a & 42m & 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] \\
\end{array}
\]

Symmetry of Special Projections

Along \([0,0,1]\) \hspace{1cm} p4mm1' \hspace{1cm} \begin{array}{c} a^* = a \\ a^* = -c \hspace{1cm} b^* = b \hspace{1cm} a^* = (a + b)/2 \hspace{1cm} b^* = c \end{array} \\
Origin at 0,0,z \hspace{1cm} Origin at x,0,0 \hspace{1cm} Origin at x,x,0 

Along \([1,0,0]\) \hspace{1cm} p_{2a} 2m'm' 

Along \([1,1,0]\) \hspace{1cm} p1m11' 

111.6.916 - 2 - 1826
Origin on \( \bar{4}2m \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) \quad & 1 \\
(2) \quad & 2 \quad 0,0,z \\
(3) \quad & \bar{4}^+ \quad 0,0,z; \quad 0,0,0 \\
(4) \quad & \bar{4}^+ \quad 0,0,z; \quad 0,0,0
\end{align*}
\]

\[
\begin{align*}
(1) \quad & (0,0,0) \\
(2) \quad & (2z,0,0,0) \\
(3) \quad & (4z,0,0,0) \\
(4) \quad & (4z^{-1},0,0,0)
\end{align*}
\]

For \((1,0,0) + \) set

\[
\begin{align*}
(1) \quad & t' (1,0,0) \\
(2) \quad & 2' \quad 1/2,0,z \\
(3) \quad & \bar{4}^+ \quad 1/2,-1/2,z; \quad 1/2,-1/2,0 \\
(4) \quad & \bar{4}^- \quad 1/2,1/2,z; \quad 1/2,1/2,0
\end{align*}
\]

\[
\begin{align*}
(1) \quad & (1,0,0) \\
(2) \quad & (2z,1,0,0)' \\
(3) \quad & (4z,1,0,0)' \\
(4) \quad & (4z^{-1},1,0,0)'
\end{align*}
\]
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>o</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x',y',z [u',v',w']</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y',x',z [v',u',w']</td>
</tr>
<tr>
<td>8</td>
<td>n</td>
<td>(5) x',y',z [u',v',w']</td>
</tr>
<tr>
<td>8</td>
<td>m</td>
<td>(6) x',y',z [u',v',w']</td>
</tr>
<tr>
<td>8</td>
<td>l</td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>k</td>
<td>(8) y',x',z [v',u',w']</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
<td>0,1/2,z [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>f</td>
<td>x,1/2,1/2 [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>0,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>1/2,1/2,2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p_{4} 4mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
</tr>
<tr>
<td>Origin at 1/2,1/2,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = b</td>
<td>b^* = c</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = (a + b)/2</td>
<td>b^* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
$\text{P}_{42m}$

111.8.918

$\text{P}_4\text{2}m$

111.8.918

Tetragonal

$\text{42m}1'$
Origin on \( \overline{4}2m \)

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y
\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & & \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
(2) & & \begin{pmatrix} 2 \\ 0 \\ 0 \\ z \end{pmatrix} \\
(3) & & \begin{pmatrix} \overline{4}^+ \\ 0 \\ 0 \\ z \end{pmatrix} \\
(4) & & \begin{pmatrix} \overline{4}^- \\ 0 \\ 0 \\ z \end{pmatrix}
\end{align*}
\]

For \((1,0,0)' + \) set

\[
\begin{align*}
(1) & & \begin{pmatrix} t' \\ 1 \\ 0 \\ 0 \end{pmatrix} \\
(2) & & \begin{pmatrix} 2' \\ 1/2 \\ 0 \\ z \end{pmatrix} \\
(3) & & \begin{pmatrix} \overline{4}'^+ \\ 1/2,-1/2,z \end{pmatrix} \\
(4) & & \begin{pmatrix} \overline{4}'^- \\ 1/2,1/2,z \end{pmatrix}
\end{align*}
\]

Generators selected

\((1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).\)

Positions

\[
\begin{array}{llllll}
\text{Multiplicity} & \text{Wyckoff letter} & \text{Site Symmetry} & \text{Coordinates} \\
16 & o & 1 & (1) x,y,z & (2) x,y,z & (3) y,x,z & (4) y,x,z \\
 & & & \text{[u,v,w]} & \text{[u,v,w]} & \text{[v,u,w]} & \text{[v,u,w]} \\
 & & & \text{(5) x,y,z} & \text{[u,v,w]} & \text{[v,u,w]} & \text{[v,u,w]} \\
8 & n & \ldots \text{m} & x,z & x,x,z & x,x,z & x,x,z \\
 & & & \text{[u,u,0]} & \text{[u,u,0]} & \text{[u,u,0]} & \text{[u,u,0]} \\
8 & m & 2\ldots & 0,1/2,z & 1/2,0,z & 1/2,0,z & 1/2,0,z \\
 & & & \text{[u,v,0]} & \text{[v,u,0]} & \text{[v,u,0]} & \text{[v,u,0]} \\
8 & l & \ldots \text{2} & x,1/2,0 & x,1/2,0 & x,1/2,0 & x,1/2,0 \\
 & & & \text{[0,v,w]} & \text{[0,v,w]} & \text{[0,v,w]} & \text{[0,v,w]} \\
8 & k & \ldots \text{2} & x,0,1/2 & x,0,1/2 & x,0,1/2 & x,0,1/2 \\
 & & & \text{[0,v,w]} & \text{[0,v,w]} & \text{[0,v,w]} & \text{[0,v,w]} \\
8 & j & \ldots & x,1/2,1/2 & x,1/2,1/2 & x,1/2,1/2 & x,1/2,1/2 \\
 & & & \text{[u,0,0]} & \text{[u,0,0]} & \text{[u,0,0]} & \text{[u,0,0]} \\
8 & i & \ldots & x,0,0 & x,0,0 & x,0,0 & x,0,0 \\
 & & & \text{[u,0,0]} & \text{[u,0,0]} & \text{[u,0,0]} & \text{[u,0,0]} \\
4 & h & \ldots \text{2mm} & 1/2,1/2,z & 1/2,1/2,z & 1/2,1/2,z & 1/2,1/2,z \\
 & & & \text{[0,0,0]} & \text{[0,0,0]} & \text{[0,0,0]} & \text{[0,0,0]} \\
4 & g & \ldots \text{2mm} & 0,0,0 & 0,0,0 & 0,0,0 & 0,0,0 \\
 & & & \text{[0,0,0]} & \text{[0,0,0]} & \text{[0,0,0]} & \text{[0,0,0]} \\
4 & f & \ldots \text{22'} & 1/2,0,1/2 & 0,1/2,1/2 & 0,1/2,1/2 & 0,1/2,1/2 \\
 & & & \text{[0,v,0]} & \text{[v,0,0]} & \text{[v,0,0]} & \text{[v,0,0]} \\
4 & e & \ldots \text{22'} & 1/2,0,0 & 1/2,0,0 & 1/2,0,0 & 1/2,0,0 \\
 & & & \text{[u,0,0]} & \text{[u,0,0]} & \text{[u,0,0]} & \text{[u,0,0]} \\
2 & d & \ldots \text{42'} & 1/2,1/2,0 & 1/2,1/2,0 & 1/2,1/2,0 & 1/2,1/2,0 \\
 & & & \text{[0,0,0]} & \text{[0,0,0]} & \text{[0,0,0]} & \text{[0,0,0]} \\
\end{array}
\]
2  c  4\textsuperscript{2}m  0,0,1/2 [0,0,0]
2  b  42\textsuperscript{m}  1/2,1/2,1/2 [0,0,0]
2  a  42\textsuperscript{m}  0,0,0 [0,0,0]

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm\textsuperscript{1}\textsuperscript{'}</th>
<th>Along [1,0,0]</th>
<th>p2mm\textsuperscript{1}\textsuperscript{'}</th>
<th>Along [1,1,0]</th>
<th>p1m11\textsuperscript{'}</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = b)</td>
<td>(b^* = c)</td>
<td>(a^* = (-a + b)/2)</td>
<td>(b^* = c)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

111.8.918 - 3 - 1831
Origin on $\overline{4}2'm'$

Asymmetric unit: $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; x \leq y$

Symmetry Operations

For $(0,0,0) +$ set

1. $1 (0,0,0)$
2. $2 \ 0,0,z$
   $2z \ 0,0,0$
3. $4' \ 0,0,z; 0,0,0$
   $4z \ 0,0,0$
4. $4' \ 0,0,z; 0,0,0$
   $4z \ 0,0,0$

For $(0,0,1)' +$ set

1. $t' (0,0,1)$
   $1 \ 0,0,1'$
2. $2' (0,0,1) \ 0,0,z$
   $2z \ 0,0,1'$
3. $4' \ 0,0,z; 0,0,1/2$
   $4z \ 0,0,1'$
4. $4' \ 0,0,z; 0,0,1/2$
   $4z \ 0,0,1'$

5. $2 \ 0,y,1/2$
   $2z \ 0,0,1'$
6. $2 \ 0,y,1/2$
   $2z \ 0,0,1'$
7. $c (0,0,1) \ x,x,z$
   $c \ 0,0,1$
   $m_{xy} \ 0,0,0$
8. $c (0,0,1) \ x,x,z$
   $c \ 0,0,1$
   $m_{xy} \ 0,0,0$
Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 n m'</td>
<td>x,x,z [u,u,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 l .2'</td>
<td>x,1/2,0 [v,w]</td>
<td>x,1/2,0 [v,w]</td>
</tr>
<tr>
<td>8 k .2</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 j .2</td>
<td>x,1/2,1/2 [u,0,0]</td>
<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>8 i .2'</td>
<td>x,0,0 [v,w]</td>
<td>x,0,0 [v,w]</td>
</tr>
<tr>
<td>4 h 2.m'm'</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 g 2.m'm'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 f 222</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 e 222'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d 42m</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>2.c 4'2m' 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 4'2m'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>2.a 4'2'm' 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>P2' 2m'm'</th>
<th>Along [1,1,0]</th>
<th>P2'* 1m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -c</td>
<td>b* = b</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,1/2,0</td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>

111.9.919 - 2 - 1833
Origin on 4'2m'

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \quad (1,0,0) \)
2. \(2 \quad 0,0,z \quad (2_z,0,0,0) \)
3. \(4' \quad 0,0,z; 0,0,0 \quad (4_z,0,0,0)' \)
4. \(4' \quad 0,0,z; 0,0,0 \quad (4_z^{-1},0,0,0)' \)

5. \(0,y,0 \quad (2,0,0,0) \)
6. \(2 \quad x,0,0 \quad (2_x,0,0,0) \)
7. \(m' \quad x,x,z \quad (m_{xy},0,0,0)' \)
8. \(m' \quad x,x,z \quad (m_{xy},0,0,0)' \)

For \((1,0,0)' + \) set

1. \(t' \quad (1,0,0) \quad (1,1,0,0)' \)
2. \(2' \quad 1/2,0,z \quad (2_z,1,0,0)' \)
3. \(4' \quad 1/2,-1/2,z; 1/2,-1/2,0 \quad (4_z,1,0,0) \)
4. \(4' \quad 1/2,1/2,z; 1/2,1/2,0 \quad (4_z^{-1},1,0,0) \)

5. \(2' \quad 1/2,y,0 \quad (2,1,0,0)' \)
6. \(2'(1,0,0) \quad x,0,0 \quad (2_x,1,0,0)' \)
7. \(g \quad (1/2,-1/2,0) \quad x+1/2,x,z \quad (m_{xy},1,0,0) \)
8. \(g \quad (1/2,1/2,0) \quad x+1/2,x,z \quad (m_{xy},1,0,0) \)
Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(1,0,0) +</th>
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</thead>
<tbody>
<tr>
<td>16</td>
<td>[u,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 n</td>
<td>[u,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 m</td>
<td>[u,v,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 l</td>
<td>[0,v,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 k</td>
<td>[u,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 j</td>
<td>[v,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 i</td>
<td>[0,u,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 h</td>
<td>[u,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 g</td>
<td>[0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 f</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 e</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 d</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 c</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] Pₜₜ 4mm

a* = a   b* = b

Origin at 0,0,z

Along [1,0,0] p2mm1'

a* = b   b* = c

Origin at x,0,0

Along [1,1,0] P₂ₓ 1m1

a* = (-a + b)/2   b* = c

Origin at x-1/4,x+1/4,0
Origin on 4'2m'

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y\]

Symmetry Operations

For \((0,0,0) + \) set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1 (0,0,0)\</td>
<td>(0,0,0,0)</td>
</tr>
<tr>
<td>(2) 2 (x,0,0) (2_1,0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>(3) 4' (x,0,0,0) (4_1,0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>(4) 4' (x,0,0,0) (4_1,0,0,0)</td>
<td>(0,0,0)</td>
</tr>
</tbody>
</table>

For \((1,0,0)' + \) set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t' (1,0,0) (1_1,0,0)</td>
<td>(1,0,0,0)</td>
</tr>
<tr>
<td>(2) 2' (1/2,0,0) (1_2,0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>(3) 4' (1/2,1/2,0,0) (2_2,1/2,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>(4) 4' (1/2,1/2,0,0) (2_2,1/2,0,0)</td>
<td>(0,0,0)</td>
</tr>
</tbody>
</table>

Generators selected

(1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 o 1</td>
<td>(1, x,y,z [u,v,w])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>8 n (..m')</td>
<td>(x,x,z [u,u,w])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>8 m 2'..</td>
<td>(0,1/2,z [u,v,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>8 l (..2')</td>
<td>(x,1/2,0 [0,v,w])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>8 k (..2')</td>
<td>(x,0,1/2 [0,v,w])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>8 j (..2')</td>
<td>(x,1/2,1/2 [0,u,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>8 i (..2')</td>
<td>(x,0,0 [u,0,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>4 h (..m'm')</td>
<td>(1/2,1/2,z [0,0,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>4 g (..m'm')</td>
<td>(0,0,z [0,0,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>4 f (..2'2')</td>
<td>(1/2,0,1/2 [0,v,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>4 e (..2'2')</td>
<td>(1/2,0,0 [u,0,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
<tr>
<td>2 d (..2'm')</td>
<td>(1/2,1/2,0 [0,0,0])</td>
<td>((0,0,0) + (1,0,0)')</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along \([0,0,1]\) \(p\,4mm\)^
\(\mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b}\)
Origin at \(0,0,z\)

Along \([1,0,0]\) \(p\,2mm\)^
\(\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}\)
Origin at \(x,0,0\)

Along \([1,1,0]\) \(p_{\overline{c}}\,1m\)
\(\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}\)
Origin at \(x-1/4, x+1/4, 0\)

2 c \(4\overline{2}m'\) 0,0,1/2 [0,0,w]
2 b \(4\overline{2}m'\) 1/2,1/2,1/2 [0,0,0]
2 a \(4\overline{2}m'\) 0,0,0 [0,0,0]
Origin on $\bar{4}1c$

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2\)

Symmetry Operations

1. \(1\)
   \(1\) \(0,0,0\)
   \(2\) \(0,0,z\)
   \(3\) \(\bar{4}^+\) \(0,0,z; 0,0,0\)
   \(4\) \(\bar{4}^-\) \(0,0,0; 0,0,0\)

2. \(2\)
   \(0,y,1/4\)
   \(2\) \(x,0,1/4\)
   \(3\) \(\bar{4}^z\) \(0,0,1/2\) \(x,x,z\)
   \(4\) \(\bar{4}^-\) \(0,0,1/2\) \(x,x,z\)

3. \(2\)
   \(0,0,1/2\)
   \(2\) \(0,0,1/2\)
   \(3\) \(\bar{4}^z\) \(0,0,1/2\) \(x,x,z\)
   \(4\) \(\bar{4}^-\) \(0,0,1/2\) \(x,x,z\)

4. \(\bar{4}^+\) \(0,0,0\)
   \(\bar{4}^-\) \(0,0,0\)

5. \(2\)
   \(0,y,1/4\)
   \(2\) \(x,0,1/4\)
   \(3\) \(\bar{4}^z\) \(0,0,1/2\) \(x,x,z\)
   \(4\) \(\bar{4}^-\) \(0,0,1/2\) \(x,x,z\)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 n 1</td>
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</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
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<tr>
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<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
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<td>1/2,0,z [0,0,w]</td>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
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<tr>
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<td>0,0,z [0,0,w]</td>
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<td>4 j .2.</td>
<td>0,y,1/4 [0,v,0]</td>
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<td>y,0,3/4 [v,0,0]</td>
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<td>x,1/2,1/4 [u,0,0]</td>
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<td>1/2,y,1/4 [0,v,0]</td>
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<td>0,x,3/4 [0,u,0]</td>
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<tr>
<td></td>
<td>0,x,3/4 [0,u,0]</td>
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<td>2 f 4..</td>
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<td>2 a 222.</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm'</th>
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<tbody>
<tr>
<td>a* = -b</td>
<td>b* = a</td>
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<tr>
<td>Origin at 0,0,z</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
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<tr>
<td>Origin at x,0,1/4</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p2c, 1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a+b)/2</td>
<td>b* = c/2</td>
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<td>Origin at x,x,0</td>
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</tbody>
</table>
Origin on $\overline{4}1c1'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $1 +$ set

(1) $1$
\[ (1)|0,0,0] \]
(2) $2 \quad 0,0,z$
\[ (2)|0,0,0] \]
(3) $\overline{4}^+ \quad 0,0,z; \quad 0,0,0$
\[ (\overline{4}|0,0,0] \]
(4) $\overline{4}^- \quad 0,0,z; \quad 0,0,0$
\[ (\overline{4}^-|0,0,0] \]

For $1' +$ set

(1) $1'$
\[ (1)|0,0,0] \]
(2) $2' \quad 0,0,z$
\[ (2')|0,0,0] \]
(3) $\overline{4}^+ \quad 0,0,z; \quad 0,0,0$
\[ (\overline{4}|0,0,0] \]
(4) $\overline{4}^- \quad 0,0,z; \quad 0,0,0$
\[ (\overline{4}^-|0,0,0] \]
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

### Positions

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<td>(3) y,x,z [0,0,0]</td>
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<td>(4) y,z+x [0,0,0]</td>
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<td>(5) x,y,z+1/2 [0,0,0]</td>
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<td>(6) x,y,z+1/2 [0,0,0]</td>
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<td>(7) y,x,z+1/2 [0,0,0]</td>
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<td>0,1/2, z [0,0,0]</td>
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<td>1/2,0, z [0,0,0]</td>
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<td>j</td>
<td>2..1'</td>
<td>0,y,1/4 [0,0,0]</td>
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<td>0,y,1/4 [0,0,0]</td>
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<td>y,0,3/4 [0,0,0]</td>
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<td>y,0,3/4 [0,0,0]</td>
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<tr>
<td>4</td>
<td>i</td>
<td>2..1'</td>
<td>x,1/2,1/4 [0,0,0]</td>
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<tr>
<td>4</td>
<td>h</td>
<td>2..1'</td>
<td>1/2,y,1/4 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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<td>e</td>
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<td>b</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
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<td>Origin at 0,0,z</td>
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<tr>
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<th>p2mm1'</th>
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<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
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<td>Origin at x,0,1/4</td>
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<tr>
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<th>p1m11'</th>
</tr>
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<tbody>
<tr>
<td>a* = (a + b)/2</td>
<td>b* = c/2</td>
</tr>
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<td>Origin at x,x,0</td>
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</table>
Origin on $\overline{4}$'1c

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $\begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix}$

(2) $\begin{pmatrix} 2 \\ 0,0,z \end{pmatrix}$

(3) $\begin{pmatrix} 4^{-} \\ 0,0,z; 0,0,0 \end{pmatrix}$

(4) $\begin{pmatrix} 4^{-} \\ 0,0,z; 0,0,0 \end{pmatrix}$

(5) $\begin{pmatrix} 2' \\ 0,y,1/4 \end{pmatrix}$

(6) $\begin{pmatrix} 2' \\ x,0,1/4 \end{pmatrix}$

(7) $\begin{pmatrix} c \\ (0,0,1/2) \end{pmatrix}$

(8) $\begin{pmatrix} c \\ (0,0,1/2) \end{pmatrix}$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<tr>
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<td>(3) $y,x,z$ [v,u,w]</td>
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<td>(4) $y,x,z$ [v,u,w]</td>
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<td>(5) $x,y,z+1/2$ [u,v,w]</td>
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<td>4 m 2..</td>
<td>$0,1/2,z$ [0,0,w]</td>
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<tr>
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<td>4 h .2'</td>
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<tr>
<td>2 d 22'..</td>
<td>$0,1/2,1/4$ [0,0,w]</td>
</tr>
<tr>
<td>2 c 22'..</td>
<td>$1/2,1/2,1/4$ [0,0,w]</td>
</tr>
<tr>
<td>2 b 22'..</td>
<td>$1/2,0,1/4$ [0,0,w]</td>
</tr>
<tr>
<td>2 a 22'..</td>
<td>$0,0,1/4$ [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [1,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = a$</td>
<td>p4m'm'</td>
<td>p2'm'm'</td>
<td>p2v, 1m'1</td>
</tr>
<tr>
<td>$b^* = b$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,1/4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$a^* = -c$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$b^* = c/2$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on \( \overline{4}1c' \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

\begin{align*}
1 & \quad (1) & 1 & \quad (5) & 2 \\
& & (1') & & (2) 0,0,0 \\
& & (1) & & (2) 0,y,1/4 \\
& & (1') & & (2') 0,0,1/4 \\
& & (1) & & (3, 4) \overline{4}1c' \quad 0,0,z; 0,0,0 \quad \overline{4}1c' \quad 0,0,z; 0,0,0 \\
& & (1') & & (4, 4') 0,0,z; 0,0,0 \\
& & (1') & & (4) 0,0,1/2 \quad (4') 0,0,1/2
\end{align*}
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>n 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w] (5) x,y,z+1/2 [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) y,x,z+1/2 [v,u,w] (8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>m 2..</td>
<td>0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 0,1/2,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>l 2..</td>
<td>1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>k 2..</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w] 0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>j .2</td>
<td>0,y,1/4 [0,v,0] 0,y,1/4 [0,v,0] y,0,3/4 [v,0,0] y,0,3/4 [v,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>i .2</td>
<td>x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] 1/2,x,3/4 [0,u,0] 1/2,x,3/4 [0,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>h .2</td>
<td>1/2,y,1/4 [0,v,0] 1/2,y,1/4 [0,v,0] y,1/2,3/4 [v,0,0] y,1/2,3/4 [v,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>g .2</td>
<td>x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] 0,x,3/4 [0,u,0] 0,x,3/4 [0,u,0]</td>
</tr>
<tr>
<td>2</td>
<td>f 4'..</td>
<td>1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>e 4'..</td>
<td>0,0,0 [0,0,0] 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>d 222.</td>
<td>0,1/2,1/4 [0,0,0] 1/2,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>c 222.</td>
<td>1/2,1/2,1/4 [0,0,0] 1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b 222.</td>
<td>1/2,0,1/4 [0,0,0] 0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 222.</td>
<td>0,0,1/4 [0,0,0] 0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm

**Along [0,0,1]**

- \( a^* = -b \)  \( b^* = a \)
- Origin at 0,0,z

**Along [1,0,0]**

- \( a^* = b \)  \( b^* = c \)
- Origin at x,0,1/4

**Along [1,1,0]**

- \( a^* = (-a + b)/2 \)  \( b^* = c/2 \)
- Origin at x,x,0

112.4.925 - 2 - 1846
Origin on $\overline{4}1c'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $\overline{4}1c'$
2. $2\overline{4}0,0,z$
3. $0,0,0$
4. $0,0,0$
5. $2\overline{4}0,y,1/4$
6. $0,0,0$
7. $0,0,0$
8. $0,0,0$

(1) $1$ 0,0,0
(2) $2$ 0,0,0
(3) $\overline{4}1c'$ 0,0,0
(4) $\overline{4}1c'$ 0,0,0
(5) $2\overline{4}0,y,1/4$
(6) $0,0,0$
(7) $0,0,0$
(8) $0,0,0$

$112.5.926 - 1 - 1847$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>0,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>x,1/2,1/4 [v,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>1/2,y,1/4 [u,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>x,0,1/4 [v,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>0,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>0,1/2,1/4 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>0,2,0,1/4 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Origin at 0,0,z

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
</tbody>
</table>

Origin at x,0,1/4

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c</td>
<td>b* = b</td>
</tr>
</tbody>
</table>

Origin at x,x,0

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
</tr>
</tbody>
</table>
**Origin** on \( \overline{4}1c \)

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \( \bar{1} \)
   - (1) \( \bar{1} (0,0,0) \)
   - (2) \( \bar{2} 0,0,z \) \( (2_z 0,0,0) \)
   - (3) \( \bar{4} \cdot 0,0,z; 0,0,0 \) \( (4_z 0,0,0) \)
   - (4) \( \bar{4} \cdot 0,0,z; 0,0,0 \) \( (4_z^{-1} 0,0,0) \)

For \((1,0,0)' + \) set

1. \( \bar{1}' \)
   - (1) \( \bar{1}' (1,0,0) \)
   - (2) \( \bar{2}' 1/2,0,z \) \( (2_z 1,0,0)' \)
   - (3) \( \bar{4}' \cdot 1/2,-1/2,z; 1/2,-1/2,0 \) \( (4_z 1,0,0)' \)
   - (4) \( \bar{4}' \cdot 1/2,1/2,z; 1/2,1/2,0 \) \( (4_z^{-1} 1,0,0)' \)

\[ 112.6.927 \]

**Tetragonal**

\[ P_4 \overline{2}c \]

\[ 112.6.927 \]

\[ \overline{4}2m1' \]

\[ P_4 \overline{2}c \]
Generators selected
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>n</th>
<th>x, y, z [u, v, w]</th>
<th>1/2, 0, z [v, u, 0]</th>
<th>0,1/2, z +1/2 [u, v, 0]</th>
<th>1/2, 0, z +1/2 [v, u, 0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>(1) x, y, z [u, v, w]</td>
<td>(3) y, x, z [v, u, w]</td>
<td>(4) y, x, z [v, u, w]</td>
<td>(5) x, y, z +1/2 [u, v, w]</td>
</tr>
<tr>
<td>8</td>
<td>(2) x, y, z [u, v, w]</td>
<td>(6) x, y, z +1/2 [u, v, w]</td>
<td>(7) y, x, z +1/2 [v, u, w]</td>
<td>(8) y, x, z +1/2 [v, u, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0, 0, 1] \( p\overline{4}m'm' \) \( a^* = a \quad b^* = b \)
Origin at 1/2, 1/2, z

Along [1, 0, 0] \( p2mm1' \) \( a^* = b \quad b^* = c \)
Origin at x, 0, 1/4

Along [1, 1, 0] \( p_{2x} \ 1m1 \) \( a^* = (-a + b)/2 \quad b^* = (-a + b + c)/2 \)
Origin at x-1/4, x+1/4, 0
Origin on \( \overline{4}1c' \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

For \((0,0,0) + \) set

1. \( \begin{pmatrix} 1 \end{pmatrix} \)
   \( \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \)

2. \( \begin{pmatrix} 2 \end{pmatrix} \)
   \( \begin{pmatrix} 0,0,z \\ (2z,0,0,0) \end{pmatrix} \)

3. \( \begin{pmatrix} 4^+ \end{pmatrix} \)
   \( \begin{pmatrix} 0,0,z; 0,0,0 \\ (4z,0,0,0)' \end{pmatrix} \)

4. \( \begin{pmatrix} 4^- \end{pmatrix} \)
   \( \begin{pmatrix} 0,0,z; 0,0,0 \\ (4z^{-1},0,0,0)' \end{pmatrix} \)

For \((1,0,0) + \) set

5. \( \begin{pmatrix} 5 \end{pmatrix} \)
   \( \begin{pmatrix} 2 \end{pmatrix} \)
   \( \begin{pmatrix} 0,y,1/4 \\ (2z,0,0,1/2) \end{pmatrix} \)

3. \( \begin{pmatrix} 3 \end{pmatrix} \)
   \( \begin{pmatrix} 0,0,1/2 \\ (4z,0,0,1/2)' \end{pmatrix} \)

4. \( \begin{pmatrix} 4 \end{pmatrix} \)
   \( \begin{pmatrix} 0,0,1/2 \\ (4z^{-1},0,0,1/2)' \end{pmatrix} \)

For \((1,0,0) + \) set

6. \( \begin{pmatrix} 6 \end{pmatrix} \)
   \( \begin{pmatrix} 2 \end{pmatrix} \)
   \( \begin{pmatrix} x,0,1/4 \\ (2z,0,0,1/2) \end{pmatrix} \)

7. \( \begin{pmatrix} 7 \end{pmatrix} \)
   \( \begin{pmatrix} 0,0,1/2 \end{pmatrix} \)
   \( \begin{pmatrix} x,x,z \\ (m_{yz},0,0,1/2)' \end{pmatrix} \)

8. \( \begin{pmatrix} 8 \end{pmatrix} \)
   \( \begin{pmatrix} 0,0,1/2 \end{pmatrix} \)
   \( \begin{pmatrix} x,x,z \\ (m_{yz},0,0,1/2)' \end{pmatrix} \)
Generators selected (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 n 1</td>
<td>(1) x,y,z</td>
<td>(2) x',y',z'</td>
</tr>
<tr>
<td>8 m 2'..</td>
<td>0,1/2,z</td>
<td>1/2,0,z</td>
</tr>
<tr>
<td>8 l 2..</td>
<td>1/2,1/2,z</td>
<td>0,1/2,z</td>
</tr>
<tr>
<td>8 k 2..</td>
<td>0,0,z</td>
<td>0,0,z+1/2</td>
</tr>
<tr>
<td>8 j .2.</td>
<td>0,y,1/4</td>
<td>y,0,3/4</td>
</tr>
<tr>
<td>8 i .2'</td>
<td>x,1/2,1/4</td>
<td>x,1/2,3/4</td>
</tr>
<tr>
<td>8 h .2'</td>
<td>1/2,y,1/4</td>
<td>y,1/2,3/4</td>
</tr>
<tr>
<td>8 g .2</td>
<td>x,0,1/4</td>
<td>x,0,3/4</td>
</tr>
<tr>
<td>4 f 4'..</td>
<td>1/2,1/2,0</td>
<td>1/2,1/2,1/2</td>
</tr>
<tr>
<td>4 e 4'..</td>
<td>0,0,0</td>
<td>0,0,1/2</td>
</tr>
<tr>
<td>4 d 2'2'</td>
<td>0,1/2,1/4</td>
<td>0,1/2,3/4</td>
</tr>
<tr>
<td>4 c 22'2'</td>
<td>1/2,1/2,1/4</td>
<td>1/2,1/2,3/4</td>
</tr>
<tr>
<td>4 b 22'2'</td>
<td>1/2,0,1/4</td>
<td>0,1/2,3/4</td>
</tr>
<tr>
<td>4 a 222.</td>
<td>0,0,1/4</td>
<td>0,0,3/4</td>
</tr>
</tbody>
</table>

Coordinates

(0,0,0) + (1,0,0)'

Symmetry of Special Projections

Along [0,0,1] p_\alpha' 4mm
a^* = a \quad b^* = b
Origin at 0,0,z

Along [1,0,0] p2mm1'
a^* = b \quad b^* = c
Origin at x,0,1/4

Along [1,1,0] p_{2\alpha'} 1m1
a^* = (-a + b)/2 \quad b^* = c/2
Origin at x-1/4,x+1/4,0
Origin on $\overline{4}1g$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x$

Symmetry Operations

(1) $1$
   
(2) $2 \quad 0,0,z$

(3) $\overline{4}^- \quad 0,0,z; \quad 0,0,0$

(4) $\overline{4}^- \quad 0,0,z; \quad 0,0,0$

(5) $2 \quad (0,1/2,0) \quad 1/4,y,0$

(6) $2 \quad (1/2,0,0) \quad x,1/4,0$

(7) $m \quad x+1/2,x,z$

(8) $g \quad (1/2,1/2,0) \quad x,x,z$

$P\overline{4}_2,m$

$\overline{4}2m$

Tetragonal

113.1.929

P$\overline{4}_2,m$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td></td>
<td></td>
</tr>
<tr>
<td>4 e .m</td>
<td>x,x+1/2,z [u,u,0]</td>
</tr>
<tr>
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<td></td>
</tr>
<tr>
<td>4 d 2..</td>
<td>0,0,z [0,0,0]</td>
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<tr>
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<td></td>
</tr>
<tr>
<td>2 c 2.mm</td>
<td>0,1/2,z [0,0,0]</td>
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<tr>
<td>2 b 4..</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
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<td></td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'gm'   Along [1,0,0] p2m'g'   Along [1,1,0] p1m11'
\( a^* = a \)  \( b^* = b \)  \( a^* = (-a + b)/2 \)  \( b^* = c \)
Origin at 0,0,0   Origin at 1/4,0   Origin at x,x,0
Origin on $\overline{4}1g'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x$

Symmetry Operations

For 1 + set

(1) 1
    (1|0,0,0)

(5) 2 (0,1/2,0) $1/4,y,0$
    (2$y_1$|1/2,1/2,0)

(2) 2 $0,0,z$
    (2$z_1$|0,0,0)

(6) 2 (1/2,0,0) $x,1/4,0$
    (2$x_1$|1/2,1/2,0)

(3) $\overline{4}^-$ $0,0,z; 0,0,0$
    (4$z_1$|0,0,0)

(4) $\overline{4}^-$ $0,0,z; 0,0,0$
    (4$z_1$|0,0,0)

(7) $m$ $x+1/2,x,z$
    (m$y_1$|1/2,1/2,0)

For 1' + set

(1) 1'$
    (1|0,0,0)'

(5) 2' (0,1/2,0) $1/4,y,0$
    (2$y_1$|1/2,1/2,0)'

(2) 2' $0,0,z$
    (2$z_1$|0,0,0)'

(6) 2' (1/2,0,0) $x,1/4,0$
    (2$x_1$|1/2,1/2,0)'

(3) $\overline{4}^-$ $0,0,z; 0,0,0$
    (4$z_1$|0,0,0)'

(4) $\overline{4}^-$ $0,0,z; 0,0,0$
    (4$z_1$|0,0,0)'

(7) $m$ $x+1/2,x,z$
    (m$y_1$|1/2,1/2,0)'

(8) g' (1/2,1/2,0) $x,x,z$
    (m$y_1$|1/2,1/2,0)'

$P\overline{4}2_1m1'$

$\overline{4}2m1'$

Tetragonal
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>1 +</td>
<td>1' +</td>
</tr>
<tr>
<td>8 f 11'</td>
<td>(1) x,y,z [0,0,0]</td>
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<tr>
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<td>(7) ȳ̄+1/2,x̄̄+1/2,z̄̄ [0,0,0]</td>
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<tr>
<td>4 d 2..1'</td>
<td>0,0,z [0,0,0]</td>
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<td>0,0,z [0,0,0]</td>
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<td>1/2,z [0,0,0]</td>
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<td>2 b 4..1'</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2 a 4..1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
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<td>1/2,1/2,0 [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1] p4gm1'  
Along [1,0,0] p2mg1'  
Along [1,1,0] p1m11'  

\( a^* = a \)  \( b^* = b \)  
\( a^* = b \)  \( b^* = c \)  
\( a^* = (a + b)/2 \)  \( b^* = c \)
Origin on 4'1g

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1; y ≤ 1/2-x

Symmetry Operations

1. 1
   (1) 0,0,0
   (2) 0,0,z
      (2z|0,0,0)
   (3) 4'1g 0,0,z; 0,0,0
      (4z|0,0,0)|
   (4) 4'1g 0,0,z; 0,0,0
      (4z|-0,0,0)|

2. 2' (0,1/2,0) 1/4,y,0
   (2y|1/2,1/2,0)

3. 2' (1/2,0,0) x,1/4,0
   (2x|1/2,1/2,0)

4. m x+1/2,x,z
   (mxy|1/2,1/2,0)

5. g (1/2,1/2,0) x,x,z
   (mxz|1/2,1/2,0)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
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<td>(3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w] (6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z [v,u,w] (8) y+1/2,x+1/2,z [v,u,w]</td>
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</tbody>
</table>

| 4            | e m x,x+1/2,z [u,u,0] x+1/2,x,z [u,u,0] x+1/2,x,z [u,u,0] |
| 4            | d 2 m 0,0,z [0,0,w] 0,0,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] |
| 2            | c 2mm 0,1/2,z [0,0,0] 1/2,0,z [0,0,0] |
| 2            | b 4 mm 0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] |
| 2            | a 4 mm 0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4g'm' a* = a  b* = b

Along [1,0,0] p2'm'g a* = b  b* = c

Along [1,1,0] p1m11' a* = (-a + b)/2  b* = c

Origin at 0,0,z Origin at x,1/4,0 Origin at x,x,0
Origin on $\bar{4}1g'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x$

Symmetry Operations

(1) 1

(1') 0,0,0

(5) 2 (0,1/2,0) 1/4,y,0

(2) 2 0,0,z

(2') 0,0,0

(2'') 0,0,0

(2''') 0,0,0

(6) 2 (1/2,0,0) x,1/4,0

(1/2,0,0)

(1/2,1/2,0)

(1/2,1/2,0)

(7) $m'$ $x+1/2,\bar{x},z$

($m_y$ $1/2,1/2,0$)

(8) $g'$ $(1/2,1/2,0) x,x,z$

($m_{xy}$ $1/2,1/2,0$)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<th>Site Symmetry</th>
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<td></td>
<td>(3) y,x,z [u,v,w]</td>
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<td>(4) y,x,z [u,v,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
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<td></td>
<td></td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>m' x,x+1/2,z [u,u,w] x,x+1/2,z [u,u,w]</td>
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<tr>
<td></td>
<td></td>
<td>x+1/2,x,z [u,u,w]</td>
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<td></td>
<td></td>
<td>x+1/2,x,z [u,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>2.. 0,0,z [0,0,w] 0,0,z [0,0,w]</td>
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<tr>
<td></td>
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<td>1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>2.m'm' 0,1/2,z [0,0,w] 1/2,0,z [0,0,w]</td>
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<tr>
<td>2</td>
<td>b</td>
<td>4'.. 0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4'.. 0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
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</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4gm</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2m'g'</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p1m'1</td>
</tr>
</tbody>
</table>

**Origin at 0,0,z**

a* = a b* = b

**Origin at x,1/4,0**

a* = b b* = c

**Origin at x,x,0**

a* = (-a + b)/2 b* = c
**Origin** on $\overline{4}1g'$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x$

**Symmetry Operations**

1. $1$
   
   $1 | 0,0,0$

2. $2 \ 0,0,z$
   
   $(2z | 0,0,0)$

3. $\overline{4}^{-} \ 0,0,z ; 0,0,0$
   
   $(4z | 0,0,0)$

4. $\overline{4}^{-} \ 0,0,z ; 0,0,0$
   
   $(4z^{-1} | 0,0,0)$

5. $2' \ (0,1/2,0) \ 1/4,y,0$
   
   $(2y | 1/2,1/2,0)$

6. $2' \ (1/2,0,0) \ x,1/4,0$
   
   $(2x | 1/2,1/2,0)$

7. $m' \ x+1/2,\overline{x},z$
   
   $(m_{x} | 1/2,1/2,0)$

8. $g' \ (1/2,1/2,0) \ x,x,z$
   
   $(m_{xy} | 1/2,1/2,0)$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>8 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u',v',w']</td>
</tr>
<tr>
<td></td>
<td>(7) y'+1/2,x+1/2,z [v',u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'g'm
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p2'm'g
\( a^* = b \quad b^* = c \)
Origin at x,1/4,0

Along [1,1,0] p1m'1
\( a^* = (-a + b)/2 \quad b^* = c \)
Origin at x,x,0
Origin on $\bar{4}1g$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad y \leq 1/2-x$

Symmetry Operations

For (0,0,0) + set

(1) $1$

(2) $2$ \quad 0,0,z

(3) $4^{-}$ \quad 0,0,z; 0,0,0

(4) $4^{-}$ \quad 0,0,z; 0,0,0

For (0,0,1)’ + set

(1) $t’$ \quad (0,0,1)

(2) $2’$ \quad (0,0,1) \quad 0,0,z

(3) $4^{-}$’ \quad 0,0,z; 0,0,1/2

(4) $4^{-}$’ \quad 0,0,z; 0,0,1/2

113.6.934 - 1 - 1863
Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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<td>(0,0,1)' +</td>
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<td>(0,0,1)</td>
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<td>0,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>4 c 2.mm</td>
<td>0,1/2,z [0,0,0]</td>
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<td>1/2,0,z [0,0,0]</td>
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| 4 b 4'..
|              | 2,1/2,1/2 [0,0,0]|
| 4 a          | 0,0,0 [0,0,w]|
|              | 1/2,1/2,0 [0,0,w]|

Symmetry of Special Projections

Along [0,0,1] p4gm1' Along [1,0,0] p21' 2m'g' Along [1,1,0] 1m11'
\[ a^* = a \quad b^* = b \] \[ a^* = b \quad b^* = c \] \[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at 0,0,z Origin at x,1/4,0 Origin at x,x,0
Origin on $\overline{4} 1g$

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1; y \leq 1/2-x$

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1) 0,0,0
(2) 2 0,0,z
    (2) 0,0,0
(5) 2 (0,1/2,0) 1/4,y,0
    (2) 1/2,1/2,2,0
(6) 2 (1/2,0,0) x,1/4,0
    (2) 1/2,1/2,2,0
(7) $m'$ x+1/2,x,z
    (m) 1/2,1/2,2,0
(8) $n$ (1/2,1/2,1) x,x,z
    (m) 1/2,1/2,2,1

For (0,0,1) + set

(1) $t$ (0,0,1)
    (1) 0,0,1
(2) $2'$ (0,0,1) 0,0,z
    (2) 0,0,1
(5) $2'$ (0,1/2,0) 1/4,y,1/2
    (2) 1/2,1/2,2,1
(6) $2'$ (1/2,0,0) x,1/4,1/2
    (2) 1/2,1/2,2,1
(7) $c$ (0,0,1) x+1/2,x,z
    (m) 1/2,1/2,2,1
(8) $n$ (1/2,1/2,1) x,x,z
    (m) 1/2,1/2,2,1

113.7.935 - 1 - 1865
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
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<tr>
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<td>(2) x’,y’,z’ [u’,v’,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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</tr>
<tr>
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<td>(4) y’,x’,z’ [v’,u’,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
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<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4gm1’</th>
<th>Along [1,0,0] p211 2m’g’</th>
<th>Along [1,1,0] p211’1m’1</th>
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<tbody>
<tr>
<td>a* = a, b* = b</td>
<td>a* = b, b* = c</td>
<td>a* = (-a + b)/2, b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,1/4,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

113.7.935 - 2 - 1866
Origin on $\overline{4}1n$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) $z=0,0,0$

(3) $\overline{4}^\gamma$ 0,0,z; 0,0,0
(3) $\overline{4}^\gamma_z$ 0,0,0

(4) $\overline{4}^\gamma$ 0,0,z; 0,0,0
(4) $\overline{4}^\gamma_z$ 0,0,0

(5) 2 (0,1/2,0) $1/4,y,1/4$
(5) (2,1/2,1/2,1/2)

(6) 2 (1/2,0,0) $x,1/4,1/4$
(6) $(2_x,1/2,1/2,1/2)$

(7) $\overline{4}^\gamma$ 0,0,1/2 $x+1/2,x,z$
(7) (m$\overline{xy},1/2,1/2,1/2$)

(8) n (1/2,1/2,1/2) $x,x,z$
(8) (m$\overline{xy},1/2,1/2,1/2$)

P4$\overline{2}$,c

Tetragonal
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<thead>
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<th>Multiplicity</th>
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<th>Coordinates</th>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>1/2,1/2,z+1/2 [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 4..</td>
<td>0,0,1/2 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2 a 4..</td>
<td>0,0,0 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'g'm
a* = a b* = b
Origin at 0,0,z

Along [1,0,0] p2m'g'
a* = b b* = c
Origin at x,1/4,1/4

Along [1,1,0] p2v,1m'1
a* = (a + b)/2 b* = c/2
Origin at x,x,0
Origin on $\overline{4}1n1'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $1 +$ set

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2 | 0,0,0)

(3) $\overline{4}^+ 0,0,z; 0,0,0$
($4_z | 0,0,0$)

(4) $\overline{4}^- 0,0,z; 0,0,0$
($4_z^{-1} | 0,0,0$)

(5) 2 (0,1/2,0) 1/4,y,1/4
(2 | 1/2,1/2,1/2)

(6) 2 (1/2,0,0) x,1/4,1/4
(2 | 1/2,1/2,1/2)

(7) c (0,0,1/2) x+1/2,x,z
($m_x | 1/2,1/2,1/2$)

(8) n (1/2,1/2,1/2) x,x,z
($m_{xy} | 1/2,1/2,1/2$)

For $1' +$ set

(1) 1'
(1 | 0,0,0)'

(2) 2' 0,0,z
(2 | 0,0,0)'

(3) $\overline{4}^{' +} 0,0,z; 0,0,0$
($4_z^{-1} | 0,0,0$')

(4) $\overline{4}^{-'} 0,0,z; 0,0,0$
($4_z^{-1} | 0,0,0$')

(5) 2' (0,1/2,0) 1/4,y,1/4
(2 | 1/2,1/2,1/2)'

(6) 2' (1/2,0,0) x,1/4,1/4
(2 | 1/2,1/2,1/2)'

(7) c' (0,0,1/2) x+1/2,x,z
($m_x | 1/2,1/2,1/2)$'

(8) n' (1/2,1/2,1/2) x,x,z
($m_{xy} | 1/2,1/2,1/2)$'
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
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<td>(3) y,x,z [0,0,0]</td>
<td>(4) y,x,z [0,0,0]</td>
</tr>
<tr>
<td>8 e 11'</td>
<td>(5) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
<td>(8) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

4 d 2..1' 0,1/2,z [0,0,0] 1/2,0,z [0,0,0] 1/2,0,z+1/2 [0,0,0] 0,1/2,z+1/2 [0,0,0]
4 c 2..1' 0,0,z [0,0,0] 0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 1/2,1/2,z+1/2 [0,0,0]
2 b 4..1' 0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]
2 a 4..1' 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4gm1' Along [1,0,0] p2mg1' Along [1,1,0] p1m11'
a* = a b* = b a* = b b* = c a* = (-a + b)/2 b* = c/2
Origin at 0,0,z Origin at x,1/4,1/4 Origin at x,x,0
Origin on $\overline{4}1\text{m}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $1$
2. $2z; 0,0,0$
3. $\overline{4}$, $0,0,0$
4. $\overline{4}$, $0,0,0$
5. $2'(0,1/2,0)$
6. $2'(1/2,0,0)$
7. $c(0,0,1/2)$
8. $n(1/2,1/2,1/2)$

$P4^{2}_1c$
$114.3.938$

$\overline{4}^{2}_2m$
$P4^{2}_1c$

Tetragonal
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4g' m'  
\( a^* = a \)  \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p2'm' g  
\( a^* = b \)  \( b^* = c \)  
Origin at x,1/4,1/4

Along [1,1,0] p2v.1m'1  
\( a^* = (-a + b)/2 \)  \( b^* = c/2 \)  
Origin at x,x,0
Origin on $\overline{4}1n'$

Asymmetric unit \[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2 \]

Symmetry Operations

(1) 1  
(2) 2 0,0,0  
(3) $\overline{4}1$' 0,0,0; 0,0,0  
(4) $\overline{4}1$' 0,0,0; 0,0,0  
(5) 2 (0,1/2,0) 1/4,y,1/4  
(6) 2 (1/2,0,0) x,1/4,1/4  
(7) $c'$ (0,0,1/2) x+1/2,x,z  
(8) n' (1/2,1/2,1/2) x,x,z

Symbols:
- \( x \), \( y \), \( z \) are translations.
- \( \overline{4} \) and \( \overline{4}1n' \) are symmetry operations.
- The asymmetric unit is given by the range of \( x, y, z \).

The diagram illustrates the crystal structure with atoms positioned according to the symmetry operations provided.
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 e 1</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(3) y, x, z [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(4) y, x, z [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(5) x + 1/2, y + 1/2, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(6) x + 1/2, y + 1/2, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(7) y + 1/2, x + 1/2, z + 1/2 [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(8) y + 1/2, x + 1/2, z + 1/2 [v, u, w]</td>
</tr>
</tbody>
</table>

4 d 2.. 0, 1/2, z [0, 0, w] 1/2, 0, z [0, 0, w] 1/2, 0, z + 1/2 [0, 0, w] 0, 1/2, z + 1/2 [0, 0, w]

4 c 2.. 0, 0, z [0, 0, w] 0, 0, z [0, 0, w] 1/2, 1/2, z + 1/2 [0, 0, w] 1/2, 1/2, z + 1/2 [0, 0, w]

2 b 4.. 0, 0, 1/2 [0, 0, 0] 1/2, 1/2, 0 [0, 0, 0]

2 a 4.. 0, 0, 0 [0, 0, 0] 1/2, 1/2, 1/2 [0, 0, 0]

Symmetry of Special Projections

Along [0, 0, 1] p4gm Along [1, 0, 0] p2m'g' Along [1, 1, 0] p1m'1

a* = a  b* = b  a* = b  b* = c  a* = (a + b)/2  b* = c/2

Origin at 0, 0, z  Origin at x, 1/4, 1/4  Origin at x, x, 0
Origin on $\overline{4}1n'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$
(1)$^*$ $0,0,0$

(2) $2$ 0,0,z
(2)$^*$ 0,0,0

(3) $\overline{4}^*$ 0,0,z; 0,0,0
(4) $\overline{4}$ 0,0,z; 0,0,0

(5) $2'$ (0,1/2,0) 1/4,y,1/4
(2)$^*$ (0,1/2,0) 1/4,y,1/4

(6) $2'$ (1/2,0,0) x,1/4,1/4
(2)$^*$ (1/2,0,0) x,1/4,1/4

(7) $c'$ (0,0,1/2) x+1/2,x,z
(m$_x$) (0,0,1/2) x+1/2,x,z

(8) n' (1/2,1/2,1/2) x,x,z
(m$_{xy}$) (1/2,1/2,1/2) x,x,z
### Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>e</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>2.. 0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 0,1/2,z+1/2 [0,0,w]</td>
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<tr>
<td>4</td>
<td>c</td>
<td>2.. 0,0,z [0,0,w] 0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4.. 0,0,1/2 [0,0,w] 1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4.. 0,0,0 [0,0,w] 1/2,1/2,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]** p4'g'm
  \[a^* = a \quad b^* = b\]
  Origin at 0,0,z

- **Along [1,0,0]** p2'm'g
  \[a^* = b \quad b^* = c\]
  Origin at x,1/4,1/4

- **Along [1,1,0]** p1m'1
  \[a^* = (-a + b)/2 \quad b^* = c/2\]
  Origin at x,x,0
Origin on $\bar{4}m2$

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

1. 1
2. 2 0,0,z
   0,0,0
3. $\bar{4}^+ \cdot 0,0,0; 0,0,0$
   $\bar{4}^- \cdot 0,0,0; 0,0,0$
4. $\bar{4}^- \cdot 0,0,0; 0,0,0$
   $\bar{4}^+ \cdot 0,0,0; 0,0,0$
5. m x,0,z
   (m_y|0,0,0)
6. m 0,y,z
   (m_x|0,0,0)
7. 2 x,x,0
   (2_{xy}|0,0,0)
8. 2 x,0
   (2_{xy}|0,0,0)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 l 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>4 k .m. x,1/2,z [0,v,0]</td>
<td>1/2,x,z [v,0,0]</td>
<td>1/2,x,z [v,0,0]</td>
</tr>
<tr>
<td>4 j .m. x,0,z [0,v,0]</td>
<td>0,x,z [v,0,0]</td>
<td>0,x,z [v,0,0]</td>
</tr>
<tr>
<td>4 i .2 x,x,1/2 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>4 h .2 x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>2 g 2mm. 0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 f 2mm. 1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
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<tr>
<td>2 e 2mm. 0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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</tr>
<tr>
<td>1 d m2 0,0,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>1 c m2 1/2,1/2,1/2 [0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>1 b m2 1/2,1/2,0 [0,0,0]</td>
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</tr>
<tr>
<td>1 a m2 0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4' mm' 
Along [1,0,0] p1m11' 
Along [1,1,0] p2m'm'

a* = a b* = b 
a* = b b* = c 
a* = (a + b)/2 b* = c
Origin on $\bar{4}m21'$

Asymmetric unit $\quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $1 +$ set

(1) 1
(1) 0,0,0)
(2) 2 0,0,z
(2z|0,0,0)
(3) $\bar{4}^+$ 0,0,z; 0,0,0
(4z|0,0,0)
(4) $\bar{4}^-$ 0,0,z; 0,0,0
(4z|0,0,0)

(5) m 0,0,0 (m_y|0,0,0)

(6) m 0,y,z
(m_x|0,0,0)
(7) 2 x,x,0
(2xy|0,0,0)
(8) 2 x,x,0
(2xy|0,0,0)

For $1' +$ set

(1) 1'
(1|0,0,0)'
(2) 2' 0,0,z
(2z|0,0,0)'
(3) $\bar{4}^+'$ 0,0,z; 0,0,0
(4z|0,0,0)'
(4) $\bar{4}^-'$ 0,0,z; 0,0,0
(4z|0,0,0)'

(5) m' x,0,z
(m_y'|0,0,0)'
(6) m' 0,y,z
(m_x'|0,0,0)'
(7) 2' x,x,0
(2xy|0,0,0)'
(8) 2' x,x,0
(2xy|0,0,0)'

115.2.942 - 1 - 1879
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

**Positions**

**Multiplicities, Wyckoff letter, Site Symmetry.**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
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<td>11'</td>
<td>1 +</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [0,0,0]</td>
<td>(6) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>.m.1'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>x,1/2,z [0,0,0]</td>
<td>x,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>.m.1'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>x,0,z [0,0,0]</td>
<td>x,0,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>.21'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [0,0,0]</td>
<td>x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>.21'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [0,0,0]</td>
<td>x,x,0 [0,0,0]</td>
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<tr>
<td>2</td>
<td>2mm.1'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>2mm.1'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
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<td>2</td>
<td>2mm.1'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>4mm21'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
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<tr>
<td>1</td>
<td>4mm21'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>1</td>
<td>4mm21'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,2 [0,0,0]</td>
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<tr>
<td>1</td>
<td>4mm21'</td>
<td>1'</td>
</tr>
<tr>
<td></td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1]  
  \[ a^* = a \quad b^* = b \]  
  Origin at 0,0,z

- Along [1,0,0]  
  \[ a^* = b \quad b^* = c \]  
  Origin at x,0,0

- Along [1,1,0]  
  \[ a^* = (-a + b)/2 \quad b^* = c \]  
  Origin at x,x,0
Origin on $\overline{4}m\bar{2}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $1$
   
   (1) $0,0,0$

2. $2 \cdot 0,0,0$

   (2) $z \cdot 0,0,0$

3. $\overline{4} \cdot 0,0,0; 0,0,0$

   (3) $\overline{4} \cdot 0,0,0$

4. $\overline{4} \cdot 0,0,0; 0,0,0$

   (4) $\overline{4} \cdot 0,0,0$

5. $m' \cdot x,0,z$

   (5) $m' \cdot 0,0,0$

   (m_y \cdot 0,0,0)$

6. $m' \cdot 0,y,z$

   (6) $m' \cdot 0,0,0$

    (m_x \cdot 0,0,0)$

7. $2 \cdot x,x,0$

   (7) $2 \cdot x,x,0$

    (2_{xy} \cdot 0,0,0$

8. $2 \cdot x,x,0$

    (8) $2 \cdot x,x,0$

    (2_{xy} \cdot 0,0,0$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
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<td>0,0,z [0,0,w]</td>
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<td>d</td>
<td>4'm'2 0,0,1/2 [0,0,0]</td>
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<tr>
<td>1</td>
<td>c</td>
<td>4'm'2 1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>1</td>
<td>b</td>
<td>4'm'2 1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>1</td>
<td>a</td>
<td>4'm'2 0,0,0 [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
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<tr>
<td>Origin at 0,0,z</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>b* = c</td>
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<tr>
<td>Origin at x,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
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</tr>
</tbody>
</table>
Origin on $\bar{4}m2'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

1. $1$  
   $1$  

2. $2$  
   $0,0,z$  
   $(2z,0,0,0)$

3. $\bar{4}$  
   $0,0,z$  
   $0,0,0$  
   $(4,0,0,0)'$

4. $\bar{4}$  
   $0,0,z$  
   $0,0,0$  
   $(4z^{-1},0,0,0)'$

5. $m$  
   $x,0,z$  
   $(m_y,0,0,0)$

6. $m$  
   $0,y,z$  
   $(m_x,0,0,0)$

7. $2'$  
   $x,x,0$  
   $(2x,0,0,0)'$

8. $2'$  
   $x,x,0$  
   $(2x,0,0,0)'$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>8 l 1</td>
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<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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<tr>
<td>4 k .m.</td>
<td>x,1/2,z [0,v,0]</td>
<td>1/2,x,z [v,0,0]</td>
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<td>x,0,z [0,v,0]</td>
<td>0,x,z [v,0,0]</td>
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</tr>
<tr>
<td>4 i ..2'</td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
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<tr>
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<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
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<td>2 g 2mm.</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
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<tr>
<td>2 f 2mm.</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
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<tr>
<td>2 e 2mm.</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<tr>
<td>1 d 4'm2'</td>
<td>0,0,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>1 c 4'm2'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>1 b 4'm2'</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>1 a 4'm2'</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [1,1,0]</th>
<th>p2'm2'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -c</td>
<td>b* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,0</td>
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</tbody>
</table>
Origin on $\bar{4}m'2'$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$

(1) $|0,0,0)$

(2) $2 \quad 0,0,z$

(2) $(2z,0,0)$

(3) $\bar{4} \quad 0,0,z; 0,0,0$

(3) $(4z,0,0)$

(4) $\bar{4} \quad 0,0,z; 0,0,0$

(4) $(4z^{-1},0,0,0)$

(5) $m' \quad x,0,z$

(5) $(m_x|0,0,0)'$

(6) $m' \quad 0,y,z$

(6) $(m_y|0,0,0)'$

(7) $2' \quad x,x,0$

(7) $(2_{xy}|0,0,0)'$

(8) $2' \quad x,x,0$

(8) $(2_{xy}|0,0,0)'$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8 l 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w] (5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>4 k .m'</td>
<td>x,1/2,z [u,0,w] x,1/2,z [u,0,w] 1/2,x,z [0,u,w] 1/2,x,z [0,u,w]</td>
</tr>
<tr>
<td>4 j .m'</td>
<td>x,0,z [u,0,w] x,0,z [u,0,w] 0,x,z [0,u,w] 0,x,z [0,u,w]</td>
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<tr>
<td>4 i .2'</td>
<td>x,x,1/2 [u,u,w] x,x,1/2 [u,u,w] x,x,1/2 [u,u,w] x,x,1/2 [u,u,w]</td>
</tr>
<tr>
<td>4 h .2'</td>
<td>x,x,0 [u,u,w] x,x,0 [u,u,w] x,x,0 [u,u,w] x,x,0 [u,u,w]</td>
</tr>
<tr>
<td>2 g 2m'm'</td>
<td>0,1/2,z [0,0,w] 1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 f 2m'm'</td>
<td>1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
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<tr>
<td>2 e 2m'm'</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1 d 4m2'</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 c 4m2'</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
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<tr>
<td>1 b 4m2'</td>
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<tr>
<td>1 a 4m2'</td>
<td>0,0,0 [0,0,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p4m'm' Along [1,0,0] p1m'1 Along [1,1,0] p2mm'
a* = a b* = b a* = b b* = c a* = -c b* = (-a + b)/2
Origin at 0,0,z Origin at x,0,0 Origin at x,x,0
Origin on \( \overline{4}m2 \)

Asymmetric unit \( 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \)

Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
2. \(2 \quad 0,0,z \quad (2z|0,0,0)\)
3. \(\overline{4}^+ \quad 0,0,z; \quad 0,0,0 \quad (4z|0,0,0)\)
4. \(\overline{4}^+ \quad 0,0,z; \quad 0,0,0 \quad (4z^{-1}|0,0,0)\)

(5) \(m \quad x,0,z \quad (m_{y}|0,0,0)\)
(6) \(m \quad 0,y,z \quad (m_{x}|0,0,0)\)
(7) \(2 \quad x,x,0 \quad (2_{xy}|0,0,0)\)
(8) \(2 \quad x,x,0 \quad (2_{xy}|0,0,0)\)

For \((0,0,1)\)' + set

1. \(t' \quad (0,0,1) \quad (1|0,0,1)\)
2. \(2' \quad (0,0,0) \quad 0,0,z \quad (2z|0,0,1)'\)
3. \(\overline{4}^+ \quad 0,0,z; \quad 0,0,1/2 \quad (4z|0,0,1)'\)
4. \(\overline{4}^+ \quad 0,0,z; \quad 0,0,1/2 \quad (4z^{-1}|0,0,1)'\)

(5) \(c' \quad (0,0,1) \quad x,0,z \quad (m_{y}|0,0,1)'\)
(6) \(c' \quad (0,0,1) \quad 0,y,z \quad (m_{x}|0,0,1)'\)
(7) \(2' \quad x,x,1/2 \quad (2_{xy}|0,0,1)'\)
(8) \(2' \quad x,x,1/2 \quad (2_{xy}|0,0,1)'\)

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Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>x,1/2,z [0,v,0]</td>
<td>x,1/2,z [0,v,0]</td>
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<td>j</td>
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<td>.m.</td>
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<td>i</td>
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<tr>
<td>.2'</td>
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<td>x,x,1/2 [u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
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<td>x,x,1/2 [u,u,w]</td>
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<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
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<td>f</td>
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<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
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<td>0,0,z [0,0,0]</td>
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<td>2</td>
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<td>d</td>
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<td>4'm2'</td>
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<td>0,0,1/2 [0,0,0]</td>
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<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm1'  
Along [1,0,0] p1m11'  
Along [1,1,0] p2a* 2m'm'

a* = a  b* = b  
a* = b  b* = c  
a* = -c  b* = (-a + b)/2

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0

115.6.946 - 2 - 1888
Origin on $\bar{4}m2$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) + \text{set}$

(1) $1$

(1) $0,0,0$

(5) $m \times 0, z$

$m_{y} | 0,0,0$

(6) $m \times 0, y$

$m_{x} | 0,0,0$

(7) $2 \times x, x$

(2) $x, x, 0$

(3) $4' \times 0,0,z; 0,0,0$

$2_{z} | 0,0,0$

(4) $4' \times 0,0,z; 0,0,0$

$2_{z}^{-1} | 0,0,0$

For $(1,0,0)' + \text{set}$

(1) $t' (1,0,0)$

(1) $1,0,0'$

(5) $a' (1,0,0) \times 0, z$

$m_{y} | 1,0,0$

(6) $m' 1/2,y,z$

$m_{x} | 1,0,0$

(7) $2' (1/2,1/2,0) \times +1/2,x$

$(2)_{y} | 0,0,0$

(3) $4' ' 1/2,-1/2,z; 1/2,-1/2,0$

$(4)_{z} | 1,0,0'$

(4) $4' ' 1/2,2,1/2,z; 1/2,1/2,0$

$(4)_{z}^{-1} | 1,0,0'$

(8) $2' (1/2,-1/2,0) \times +1/2,x$

$(2)_{y} | 0,0,0$

$\bar{4}m2$

115.7.947

Tetragonal

P$_{4}$ $\bar{4}m2$

$115.7.947 - 1 - 1889$
Generators selected
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>16 l</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 k .m'</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>8 j .m</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>8 i ..2</td>
<td>x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td>8 h ..2</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>4 g 2'm'</td>
<td>0,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>4 f 2m'm'</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 2mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d 4m2</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 4'm2</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 4'm2</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 4m2</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{c}4m'm' \) Along [1,0,0] \( p1m11' \) Along [1,1,0] \( p_{2a}2m'm' \)
\( a^* = a \quad b^* = b \)
\( a^* = b \quad b^* = c \)
Origin at 0,0,z Origin at x,0,0 Origin at x,x,0
Origin on $\bar{4}m2$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$ (1) $0,0,0$
2. $2$ $0,0,z$ (2z $0,0,0$
3. $\bar{4}^{-1}$ $0,0,z$; $0,0,0$ (4z $0,0,0$
4. $\bar{4}^{-1}$ $0,0,z$; $0,0,0$ ($4z^{-1}$ $0,0,0$

(5) m $x,0,z$
(m$_{y}$ $0,0,0$

(6) m $0,y,z$
(m$_{x}$ $0,0,0$

(7) 2 $x,x,0$
($2_{xy}$ $0,0,0$

(8) 2 $x,x,0$
($2_{xy}$ $0,0,0$

For $(1,0,0)'$ + set

1. $t'(1,0,0)$ (1) $1,0,0$
2. $2'$ $1/2,0,z$ (2z $1,0,0$
3. $\bar{4}^{-1}$ $1/2,-1/2,z$; $1/2,-1/2,0$ (4z $1,0,0$
4. $\bar{4}^{-1}$ $1/2,1/2,z$; $1/2,1/2,0$ ($4z^{-1}$ $1,0,0$

(5) a' $(1,0,0)$ $x,0,z$
(m$_{y}$ $1,0,0$

(6) m' $1/2,y,z$
(m$_{x}$ $1,0,0$

(7) 2' $(1/2,1/2,0)$ $x+1/2,x,0$
($2_{xy}$ $1,0,0$

(8) 2' $(1/2,-1/2,0)$ $x+1/2,x,0$
($2_{xy}$ $1,0,0$

Generators selected (1); $t'(1,0,0)$; $t'(0,1,0)$; $t'(0,0,1)$; (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

(0,0,0) +

1. $1$ $x,y,z$ [u,v,w]$\quad (1)$ $\bar{x},\bar{y},\bar{z}$ [u,v,w]$\quad (2)$ $\bar{x},\bar{y},z$ [u,v,w]$\quad (3)$ $y,x,z$ [u,v,w]$\quad (4)$ $y,x,z$ [v,u,w]

(5) $x,y,z$ [u,v,w]$\quad (6)$ $x,y,z$ [u,v,w]$\quad (7)$ $y,x,z$ [v,u,w]$\quad (8)$ $y,x,z$ [v,u,w]

8. k $0.1/2,0,[u,0,0]$ $\bar{x},1/2,z$ [u,0,0]$\quad 1/2,\bar{x},z$ [0,u,w]$\quad 1/2,\bar{x},z$ [0,u,w]

8. j $0.0,0,[0,v,0]$ $\bar{x},0,z$ [0,0,0]$\quad 0,\bar{x},z$ [v,0,0]$\quad 0,\bar{x},z$ [v,0,0]

8. i $0.1/2$ $x,x,1/2$ [u,u,w]$\quad \bar{x},x,1/2$ [u,u,w]$\quad x,x,1/2$ [u,u,w]$\quad \bar{x},x,1/2$ [u,u,w]

8. h $0.0,0,[u,0,0]$ $\bar{x},x,0$ [u,u,0]$\quad x,\bar{x},0$ [u,u,0]$\quad \bar{x},x,0$ [u,u,0]

4. g $20.1/2,0,[0,0,0]$ $1/2,0,z$ [u,0,0]$\quad 1/2,0,z$ [0,u,0]

4. f $20.1/2,0,[0,0,0]$ $1/2,1/2,z$ [0,0,w]$\quad 1/2,1/2,z$ [0,0,w]

4. e $20.0,0,[0,0,0]$ $0,0,z$ [0,0,0]$\quad 0,0,z$ [0,0,0]

2. d $\bar{4}m2'$ $0.0,1/2$ [0,0,0]$\quad 0.0,1/2$ [0,0,0]

2. c $\bar{4}m2'$ $1/2,1/2,1/2$ [0,0,w]$\quad 1/2,1/2,1/2$ [0,0,w]

2. b $\bar{4}m2'$ $1/2,1/2,0$ [0,0,0]$\quad 1/2,1/2,0$ [0,0,0]

2. a $\bar{4}m2$ $0.0,0$ [0,0,0]$\quad 0.0,0$ [0,0,0]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p 4mm1'</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p1m11'</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>a* = b</td>
<td>b* = c</td>
<td></td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p_c 2mm</td>
<td>Origin at x-1/4,x+1/4,1/2</td>
</tr>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
<td></td>
</tr>
</tbody>
</table>
P2c 4m2

Tetragonal

115.9.949

\( m \) 2

Asymmetric unit

\[ 0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2} \]

\textbf{Symmetry Operations}

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(1) & \quad (0,0,0) \\
(5) & \quad m' x,0,z \\
(5) & \quad (m_x | 0,0,0)' \\
(5) & \quad (m_y | 0,0,0)' \\
(6) & \quad m' 0,y,z \\
(6) & \quad (m_y | 0,0,0)' \\
(6) & \quad (m_x | 0,0,0)' \\
(7) & \quad 2' \quad 0,0,z \\
(7) & \quad (2_z | 0,0,0)' \\
(7) & \quad (2_y | 0,0,0) \\
(7) & \quad (2_x | 0,0,0) \\
(8) & \quad 2' \quad 0,0,z \\
(8) & \quad (2_z | 0,0,0)' \\
(8) & \quad (2_y | 0,0,0) \\
(8) & \quad (2_x | 0,0,0)' \\
(1) & \quad t' \quad (0,0,1) \\
(1) & \quad (0,0,1)' \\
(1) & \quad (0,0,1)' \\
(5) & \quad c (0,0,1) \quad x,0,z \\
(5) & \quad (m_x | 0,0,1) \\
(5) & \quad (m_y | 0,0,1)' \\
(6) & \quad c (0,0,1) \quad 0,y,z \\
(6) & \quad (m_x | 0,0,1) \\
(6) & \quad (m_y | 0,0,1)' \\
(7) & \quad 2' \quad x,x,1/2 \\
(7) & \quad (2_x | 0,0,1)' \\
(7) & \quad (2_y | 0,0,1)' \\
(8) & \quad 2' \quad x,x,1/2 \\
(8) & \quad (2_x | 0,0,1)' \\
(8) & \quad (2_y | 0,0,1)' \\
\end{align*}

\textbf{Origin on \( \overline{4} \)'m'2}

For \((0,0,0)\) set

\begin{align*}
(1) \quad & \quad 1 \\
(2) \quad & \quad 2 \quad 0,0,z \\
(2) \quad & \quad (2_z | 0,0,0) \\
(3) \quad & \quad 4^+ \quad 0,0,z; \quad 0,0,0 \\
(3) \quad & \quad (4_z | 0,0,0)' \\
(4) \quad & \quad 4^+ \quad 0,0,z; \quad 0,0,0 \\
(4) \quad & \quad (4_z |-1,0,0)' \\
\end{align*}

For \((0,0,1)\) set

\begin{align*}
(1) \quad & \quad t' \quad (0,0,1) \\
(1) \quad & \quad (0,0,1)' \\
(2) \quad & \quad 2' \quad (0,0,1) \quad 0,0,z \\
(2) \quad & \quad (2_z | 0,0,1)' \\
(3) \quad & \quad 4^+ \quad 0,0,z; \quad 0,0,1/2 \\
(3) \quad & \quad (4_z | 0,0,1) \\
(4) \quad & \quad 4^+ \quad 0,0,z; \quad 0,0,1/2 \\
(4) \quad & \quad (4_z |-1,0,1) \\
(5) \quad & \quad c (0,0,1) \quad x,0,z \\
(5) \quad & \quad (m_x | 0,0,1) \\
(6) \quad & \quad c (0,0,1) \quad 0,y,z \\
(6) \quad & \quad (m_x | 0,0,1) \\
(7) \quad & \quad 2' \quad x,x,1/2 \\
(7) \quad & \quad (2_x | 0,0,1)' \\
(8) \quad & \quad 2' \quad x,x,1/2 \\
(8) \quad & \quad (2_x | 0,0,1)' \\
\end{align*}
Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>16</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>k .m'. x,1/2,z [u,0,w]</td>
</tr>
<tr>
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<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,x,z [0,u,w]</td>
</tr>
<tr>
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<td>1/2,x,z [0,u,w]</td>
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<tr>
<td>8</td>
<td>j .m'. x,0,z [u,0,w]</td>
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<tr>
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<tr>
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<td>0,x,z [0,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>i ..2' x,x,1/2 [u,u,w]</td>
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<td>x,x,1/2 [u,u,w]</td>
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<tr>
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<td>x,x,1/2 [u,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>h ..2 x,x,0 [u,u,0]</td>
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<td></td>
<td>x,x,0 [u,u,0]</td>
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<tr>
<td>4</td>
<td>g 2m'm'. 0,1/2,z [0,0,w]</td>
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<td>1/2,0,z [0,0,w]</td>
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<tr>
<td>4</td>
<td>f 2m'm'. 1/2,1/2,z [0,0,w]</td>
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<td>1/2,1/2,z [0,0,w]</td>
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<tr>
<td>4</td>
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<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>d 4m'2' 0,0,1/2 [0,0,w]</td>
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<tr>
<td>2</td>
<td>c 4m'2' 1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 4m'2' 1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 4m'2' 0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>p2a1m1'</th>
<th>Along [1,1,0]</th>
<th>p2a1m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -c</td>
<td>b* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
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<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,1/2</td>
<td></td>
</tr>
</tbody>
</table>
Origin on $\overline{4}m2'$

Asymmetric unit 

$0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2$

Symmetry Operations

For (0,0,0) + set

(1) $1$
(1) $0,0,0$

(2) $2' \quad 0,0,z$
(2) $z,0,0,0$

(3) $\overline{4} +' \quad 0,0,z; \quad 0,0,0$
(4) $\overline{4} +' \quad 0,0,z; \quad 0,0,0$

For (1,0,0)' + set

(1) $t' \quad (1,0,0)$
(1) $1,0,0$

(2) $2' \quad 1/2,0,z$
(2) $z,1,0,0$

(3) $\overline{4} +' \quad 1/2,-1/2,z; \quad 1/2,-1/2,0$
(4) $\overline{4} +' \quad 1/2,1/2,z; \quad 1/2,1/2,0$

(5) $a' \quad (1,0,0)$
(5) $x,0,z$

(6) $m' \quad 1/2,y,z$
(6) $m,1,0,0$

(7) $2' (1/2,1/2,0) \quad x+1/2,x,0$
(7) $2 (1/2,-1/2,0) \quad x+1/2,x,0$

(8) $2 (1/2,-1/2,0) \quad x+1/2,x,0$
(8) $2 (1/2,1/2,0) \quad x+1/2,x,0$
Generators selected

(1); \( t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5). 

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 l 1</td>
<td>((0,0,0) + (1,0,0)' + )</td>
<td></td>
</tr>
<tr>
<td>8 k .m'</td>
<td>((1) x,y,z [u,v,w] )</td>
<td></td>
</tr>
<tr>
<td>8 j .m</td>
<td>((2) \tilde{x},y,z [\tilde{u},\tilde{v},\tilde{w}] )</td>
<td></td>
</tr>
<tr>
<td>8 i .2</td>
<td>((3) y,x,z [\tilde{v},u,w] )</td>
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<tr>
<td>8 h .2</td>
<td>((4) y,x,z [v,u,w] )</td>
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</tr>
<tr>
<td>4 g 2mm'</td>
<td>((5) x,y,z [u,v,w] )</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 f 2m'm'</td>
<td>((6) \tilde{x},y,z [\tilde{u},\tilde{v},\tilde{w}] )</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 2mm</td>
<td>((7) y,x,z [\tilde{v},u,w] )</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d ( \bar{4}m2' )</td>
<td>((8) \tilde{y},x,z [v,u,w] )</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 c ( \bar{4}m2' )</td>
<td>((1) x,1/2,z [u,0,w] )</td>
<td>1/2,x,1/2 [u,0,0]</td>
</tr>
<tr>
<td>2 b ( \bar{4}m2' )</td>
<td>((2) \tilde{x},x,0 [u,u,0] )</td>
<td>x,x,1/2 [u,u,0]</td>
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<td>2 a ( \bar{4}m2' )</td>
<td>((3) x,y,1/2 [u,v,0] )</td>
<td>x,x,1/2 [u,u,0]</td>
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<td>((4) x,0,z [0,v,0] )</td>
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<td></td>
<td>((8) x,0,z [0,v,0] )</td>
<td>0,x,z [v,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \( p_{\beta}, 4mm \)  
Along \([1,0,0]\) \( p1m11' \)  
Along \([1,1,0]\) \( p_{2\alpha}, 2mm \)

\( a^* = a \quad b^* = b \)  
\( a^* = b \quad b^* = c \)  
\( a^* = (-a+b)/2 \quad b^* = c \)  

Origin at 1/2,1/2,z  
Origin at x,0,0  
Origin at x-1/4,x+1/4,0
Origin on $\overline{4}c1$

Asymmetric unit \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4\]

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
 & \quad (1) \ 0,0,0 \\
(2) & \quad 2 \ 0,0,z \\
 & \quad (2z) \ 0,0,0 \\
(3) & \quad \overline{4}^+ \ 0,0,z; 0,0,0 \\
 & \quad (4z) \ 0,0,0 \\
(4) & \quad \overline{4} - \ 0,0,z; 0,0,0 \\
 & \quad (4z^{-1}) \ 0,0,0 \\
(5) & \quad c \ (0,0,1/2) \ x,0,z \\
 & \quad (m_y) \ 0,0,1/2 \\
(6) & \quad c \ (0,0,1/2) \ 0,y,z \\
 & \quad (m_x) \ 0,0,1/2 \\
(7) & \quad 2 \ x,x,1/4 \\
 & \quad (2_{xy}) \ 0,0,1/2 \\
(8) & \quad 2 \ x,x,1/4 \\
 & \quad (2_{xy}) \ 0,0,1/2
\end{align*}
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>x, y, z</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1</td>
<td>1</td>
<td>x, y, z [u, v, w]</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) y, x, z [v, u, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) y, x, z [v, u, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) y, x, z [v, u, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) x, y, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(6) x, y, z+1/2 [u, v, w]</td>
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<td>(7) x, y, z+1/2 [v, u, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(8) y, x, z+1/2 [v, u, w]</td>
</tr>
<tr>
<td>4 i 2..</td>
<td>1/2,0, z [0,0,w]</td>
<td>1/2,0, z [0,0,w]</td>
<td>1/2,0, z+1/2 [0,0,w]</td>
</tr>
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<td></td>
<td></td>
<td>1/2,0, z+1/2 [0,0,w]</td>
</tr>
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<td>4 h 2..</td>
<td>1/2,1/2, z [0,0,w]</td>
<td>1/2,1/2, z [0,0,w]</td>
<td>1/2,1/2, z+1/2 [0,0,w]</td>
</tr>
<tr>
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<td></td>
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<td>1/2,1/2, z+1/2 [0,0,w]</td>
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<tr>
<td>4 g 2..</td>
<td>0,0, z [0,0,w]</td>
<td>0,0, z [0,0,w]</td>
<td>0,0, z+1/2 [0,0,w]</td>
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<td></td>
<td></td>
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<td>0,0, z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 f ..2</td>
<td>x,x,3/4 [u, u, 0]</td>
<td>x,x,3/4 [u, u, 0]</td>
<td>x,x,1/4 [u, u, 0]</td>
</tr>
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<td>x,x,3/4 [u, u, 0]</td>
</tr>
<tr>
<td>2 d 4</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c 4</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 2.22</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td></td>
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<tr>
<td>2 a 2.22</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'mm'  
Along [1,0,0] p2b1m'1  
Along [1,1,0] p2m'm'

\( a^* = a \quad b^* = b \)  
Origin at 0,0,z  
\( a^* = b \quad b^* = c/2 \)  
Origin at x,0,0  
\( a^* = (a + b)/2 \quad b^* = c \)  
Origin at x,x,1/4
Origin on $\overline{4}c1'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

(1) 1

(1) 0,0,0

(5) $c (0,0,1/2) \cdot x,0,z$

(6) $c (0,0,1/2) \cdot 0,y,z$

(7) $2' \cdot x,x,1/4$

(8) $2' \cdot x,x,1/4$

For 1' + set

(1) 1'

(1) 0,0,0'

(5) $c' (0,0,1/2) \cdot x,0,z$

(6) $c' (0,0,1/2) \cdot 0,y,z$

(7) $2' \cdot x,x,1/4$

(8) $2' \cdot x,x,1/4$
GENERATORS

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

POSITIONS

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) (\bar{x},\bar{y},\bar{z}) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y,(\bar{x},\bar{z}) [0,0,0]</td>
<td>(4) y,(\bar{x},\bar{z}) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) x,(\bar{y},\bar{z}+1/2) [0,0,0]</td>
<td>(6) (\bar{x},\bar{y},\bar{z}+1/2) [0,0,0]</td>
</tr>
<tr>
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<td>(7) y,(\bar{x},\bar{z}+1/2) [0,0,0]</td>
<td>(8) y,(\bar{x},\bar{z}+1/2) [0,0,0]</td>
</tr>
<tr>
<td>4 i 2..1'</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
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<td>0,1/2,z+1/2 [0,0,0]</td>
<td>1/2,0,z+1/2 [0,0,0]</td>
</tr>
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<td>4 h 2..1'</td>
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</tr>
<tr>
<td>4 g 2..1'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
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<td>0,0,z+1/2 [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
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<tr>
<td>4 f ..21'</td>
<td>x,x,3/4 [0,0,0]</td>
<td>x,x,1/4 [0,0,0]</td>
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<tr>
<td></td>
<td>x,x,3/4 [0,0,0]</td>
<td>x,x,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 e ..21'</td>
<td>x,x,1/4 [0,0,0]</td>
<td>x,x,1/4 [0,0,0]</td>
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<td></td>
<td>x,x,3/4 [0,0,0]</td>
<td>x,x,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 d (\bar{4})1'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c (\bar{4})1'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 2.221'</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 a 2.221'</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

SYMMETRY OF SPECIAL PROJECTIONS

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Origin at x,0,0</th>
<th>Origin at x,x,1/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a) (b^* = b)</td>
<td>(a^* = b) (b^* = c/2)</td>
<td>(a^* = -(a + b)/2) (b^* = c)</td>
</tr>
</tbody>
</table>
Origin on $\overline{4}c'1$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $\overline{4}c'2$

2. $\overline{4}m'2$ Tetragonal

$P\overline{4}c'2$

$116.3.953$

$\overline{4}m'2$

$P\overline{4}c'2$

Symmetry Operations:

1. $1 \quad (0,0,0)$

2. $2 \quad 0,0,z \quad (2z,0,0,0)$

3. $\overline{4}c' \quad 0,0,z; 0,0,0 \quad (\overline{4}z,0,0,0')$

4. $\overline{4}c' \quad 0,0,z; 0,0,0 \quad (\overline{4}z,1,0,0')$

5. $c' \quad (0,0,1/2); \quad x,0,z \quad (m_y,0,0,1/2)'$

6. $c' \quad (0,0,1/2); \quad 0,y,z \quad (m_x,0,0,1/2)'$

7. $2 \quad x,x,1/4 \quad (2y,0,0,1/2)$

8. $2 \quad x,x,1/4 \quad (2y,0,0,1/2)$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 j 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>4 i 2. 0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 h 2. 1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 g 2. 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 f ..2 x,x,3/4 [u,u,0]</td>
<td>x,x,3/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td>4 e ..2 x,x,1/4 [u,u,0]</td>
<td>x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,3/4 [u,u,0]</td>
</tr>
<tr>
<td>2 d 4. 1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 4. 0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 2.22 1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
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<tr>
<td>2 a 2.22 0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p4m'm'</th>
<th>Along [1,0,0] p1m'</th>
<th>Along [1,1,0] p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a   b' = b</td>
<td>a' = b   b' = c/2</td>
<td>a' = (-a + b)/2   b' = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,1/4</td>
</tr>
</tbody>
</table>

116.3.953 - 2 - 1903
Origin on $\overline{4}c1$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $\overline{4}c2'$
   - $0,0,0$
   - $0,0,0$

2. $2\overline{4}c2'$
   - $2,0,z$
   - $2,0,0$

3. $\overline{4}c2'$
   - $0,0,z$
   - $0,0,0$

4. $\overline{4}c2'$
   - $0,0,z$
   - $0,0,0$

5. $c$ (0,0,1/2)
   - $x,0,z$
   - $(m_y,0,0,1/2)$

6. $c$ (0,0,1/2)
   - $0,y,z$
   - $(m_x,0,0,1/2)$

7. $2'$
   - $x,x,1/4$
   - $(2_{xy},0,0,1/2)$

8. $2'$
   - $x,x,1/4$
   - $(2_{xy},0,0,1/2)$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

<table>
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<tr>
<td>2 d 4'</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 c 4'</td>
<td>0,0,0 [0,0,0]</td>
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<tr>
<td>2 b 2.2'2'</td>
<td>1/2,1/2,1/4 [0,0,w]</td>
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<tr>
<td>2 a 2.2'2'</td>
<td>0,0,1/4 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm

a* = a b* = b
Origin at 0,0,z

Along [1,0,0] p21m'1

a* = b b* = c/2
Origin at x,0,0

Along [1,1,0] p2'mm'

a* = -c b* = (-a + b)/2
Origin at x,x,1/4
Origin on $\overline{4}c'1$

Asymmetric unit $\quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $1$
   - $(1,0,0)$
   - $(2z,0,0,0)$

2. $2$ $0,0,z$
   - $(0,0,0,0)$

3. $\overline{4}$ $0,0,z; 0,0,0$
   - $(0,0,0,0)$
   - $(0,0,0,0)$

4. $\overline{4}$ $0,0,z; 0,0,0$
   - $(0,0,0,0)$
   - $(0,0,0,0)$

5. $c'$ $(0,0,1/2)$ $x,0,z$
   - $(m_y,0,0,1/2)$
   - $(0,0,0,1/2)$

6. $c'$ $(0,0,1/2)$ $0,y,z$
   - $(m_x,0,0,1/2)$
   - $(0,0,0,1/2)$

7. $2'$ $x,x,1/4$
   - $(2x,0,0,1/2)$
   - $(2y,0,0,1/2)$

8. $2'$ $x,x,1/4$
   - $(2x,0,0,1/2)$
   - $(2y,0,0,1/2)$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

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<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
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Symmetry of Special Projections

- Along [0,0,1] p4'm'm
- Along [1,0,0] p1m'1
- Along [1,1,0] p2'mm'

Origin at 0,0,z

- a' = a
- b* = b

Origin at x,0,0

- a' = -c
- b* = (-a + b)/2

Origin at x,x,1/4
Origin on $\overline{4}c1$

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{4} \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad \overline{4}^+ \quad 0,0,z; 0,0,0 \\
(4) & \quad \overline{4}^+ \quad 0,0,z; 0,0,0 \\
& \quad (\overline{4}_z^\perp|0,0,0) \\
(5) & \quad c \quad (0,0,1/2) \quad x,0,z \\
& \quad (m_y|0,0,1/2) \\
(6) & \quad c \quad (0,0,1/2) \quad 0,y,z \\
& \quad (m_x|0,0,1/2) \\
(7) & \quad 2 \quad x,x,1/4 \\
& \quad (2_{xy}|0,0,1/2) \\
(8) & \quad 2 \quad x,x,1/4 \\
& \quad (2_{xy}|0,0,1/2)
\end{align*}
\]

For \((1,0,0) + \) set

\[
\begin{align*}
(1) & \quad t' \quad (1,0,0) \\
& \quad (1|1,0,0)' \\
(2) & \quad 2' \quad 1/2,0,z \\
& \quad (2_z|1,0,0)' \\
(3) & \quad \overline{4}^+ \quad 1/2,-1/2,z; 1/2,-1/2,0 \\
& \quad (\overline{4}_z|1,0,0)' \\
(4) & \quad \overline{4}^+ \quad 1/2,1/2,z; 1/2,1/2,0 \\
& \quad (\overline{4}_z^\perp|1,0,0)' \\
(5) & \quad n' \quad (1,0,1/2) \quad x,0,z \\
& \quad (m_y|1,0,1/2)' \\
(6) & \quad c' \quad (0,0,1/2) \quad 1/2,y,z \\
& \quad (m_x|1,0,1/2)' \\
(7) & \quad 2' \quad (1/2,1/2,0) \quad x+1/2,x,1/4 \\
& \quad (2_{xy}|1,0,1/2)' \\
(8) & \quad 2' \quad (1/2,-1/2,0) \quad x+1/2,x,1/4 \\
& \quad (2_{xy}|1,0,1/2)'
\end{align*}
\]
Generators selected

(1): t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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Symmetry of Special Projections

Along [0,0,1] pₚ 4m’m’

Along [1,0,0] p1m11’

Along [1,1,0] p₂a’ 2m’m’

a’ = a  b’ = b

a’ = b  b’ = c/2

a’ = (-a + b)/2  b’ = c

Origin at 1/2,1/2,z

Origin at x,0,0

Origin at x,x,1/4
Origin on \( \overline{4} \cdot c1 \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

For \((0,0,0) + \) set

1. \((1) \quad 1 \quad 0,0,0 \)
2. \((2) \quad 2'y \quad 0,0,z \quad (2z, 0, 0, 0) \)
3. \((3) \quad 2'y' \quad 0,0,0; 0,0,0 \quad (4z, 0, 0, 0) \)
4. \((4) \quad 2'y' \quad 0,0,0; 0,0,0 \quad (4z^{-1}, 0, 0, 0) \)

For \((1,0,0) + \) set

1. \((1) \quad t' \quad (1,0,0) \quad (1,1,0,0) \)
2. \((2) \quad 2'y' \quad 1/2,0,z \quad (2z, 1, 0, 0) \)
3. \((3) \quad 2'y' \quad 1/2,1/2,z; 1/2,1/2,0 \quad (4z, 1, 0, 0) \)
4. \((4) \quad 2'y' \quad 1/2,1/2,z; 1/2,1/2,0 \quad (4z^{-1}, 1, 0, 0) \)

For \((1,0,1/2) + \) set

1. \((5) \quad n' \quad (1,0,1/2) \quad x,0,z \quad (m, 0, 0, 1/2) \)
2. \((6) \quad c' \quad (0,0,1/2) \quad 0,y,z \quad (m, 0, 0, 1/2) \)
3. \((7) \quad 2'y' \quad x,x,1/4 \quad (2xy, 0, 0, 1/2) \)
4. \((8) \quad 2'y' \quad x,x,1/4 \quad (2xy, 0, 0, 1/2) \)
Generators selected

(1); t'(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>0,0,z [0,0,w]</td>
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<td>x,x,1/4 [u,u,w]</td>
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<td>0,0,1/4 [0,0,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p_p' 4mm
\[ a^* = a, \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p1m11'
\[ a^* = b, \quad b^* = c/2 \]
Origin at x,0,0

Along [1,1,0] p_{2z} 2mm
\[ a^* = (-a + b)/2, \quad b^* = c \]
Origin at x-1/4,x+1/4,1/4
Origin on $\overline{4}1_{1}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

(1) $1$
(2) $2 \quad 0,0,z$
(3) $\overline{4} \times 0,0,z; 0,0,0$
(4) $\overline{4} \times 0,0,z; 0,0,0$ $z$

(5) $a (1/2,0,0) \quad x,1/4,z$
(6) $b (0,1/2,0) \quad 1/4,y,z$
(7) $2 (1/2,1/2,0) \quad x,x,0$
(8) $2 \quad x, x+1/2,0$

$P4b2$

$\overline{4}m2$

Tetragonal
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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| (2) x,y,z [u,v,w] |
| (3) y,x,z [v,u,w] |
| (4) y,x,z [v,u,w] |
| (5) x+1/2,y+1/2,z [u,v,w] |
| (6) x+1/2,y+1/2,z [u,v,w] |
| (7) y+1/2,x+1/2,z [v,u,w] |
| (8) y+1/2,x+1/2,z [v,u,w] |

| 4            | h           |

| .2           | x,x+1/2,1/2 [u,u,0] |
| x,x+1/2,1/2 [u,u,0] |
| x,x+1/2,0 [u,u,0] |
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| 0,0,0 [0,0,0] |
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| 1/2,0,0 [0,0,0] |
| 0,0,1/2 [0,0,0] |
| 1/2,1/2,1/2 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4gm'  
Along [1,0,0] p2a1m1  
Along [1,1,0] p2m1m'  

**a** = a  
**b** = b  
**a** = b/2  
**b** = c  
**a** = (-a + b)/2  
**b** = c  
Origin at 0,0,z  
Origin at x,1/4,0  
Origin at x,x,0
**Origin** on $\bar{4}12, 1'$

**Asymmetric unit**  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

For $1 +$ set

1. $1$  
   
   \[ (1) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \]

2. $2$  
   
   \[ (2) \begin{pmatrix} 2, 0, 0, z \\ 0, 0, 0 \end{pmatrix} \]

3. $\bar{4}$  
   
   \[ (3) \begin{pmatrix} 4, 0, z; 0, 0, 0 \\ 4_z, 0, 0, 0 \end{pmatrix} \]

4. $\bar{4}$  
   
   \[ (4) \begin{pmatrix} 0, 0, z; 0, 0, 0 \\ 4_z, 0, 0, 0 \end{pmatrix} \]

For $1' +$ set

1. $1'$  
   
   \[ (1) \begin{pmatrix} 1, 0, 0, 0 \end{pmatrix} \]

2. $2'$  
   
   \[ (2) \begin{pmatrix} 2', 0, 0, z \\ 2_z, 0, 0, 0 \end{pmatrix} \]

3. $\bar{4}'$  
   
   \[ (3) \begin{pmatrix} 4', 0, z; 0, 0, 0 \\ 4_z, 0, 0, 0 \end{pmatrix} \]

4. $\bar{4}'$  
   
   \[ (4) \begin{pmatrix} 0, 0, z; 0, 0, 0 \\ 4_z, 0, 0, 0 \end{pmatrix} \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

1 + 1' +

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Symmetry of Special Projections

Along [0,0,1] p4gm1'  Along [1,0,0] p1m11'  Along [1,1,0] p2mm1'
a* = a  b* = b  a* = a/2  b* = c  a* = (a + b)/2  b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
Origin on $\overline{4}121$,

Asymmetric unit 

$$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$$

Symmetry Operations

(1) 1

(1) $0,0,0$

(1) $0,0,0$

(2) $0,0,0$

(3) $0,0,0$

(4) $0,0,0$

(5) $a'$ (1/2,0,0) 

(6) $b'$ (0,1/2,0) 

(7) $2 (1/2,1/2,0)$ 

(8) $2 x,x+1/2,0$

$\overline{4}m'$

$P\overline{4}b'$

$117.3.960$

$P\overline{4}b'$

Tetragonal
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

### Positions

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<tr>
<td>4 f 2..</td>
<td>0,1/2,z [0,0,w]</td>
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<td>1/2,0,z [0,0,w]</td>
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<td>0,1/2,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>1/2,1/2,z [0,0,w]</td>
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<td>1/2,1/2,z [0,0,w]</td>
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<tr>
<td>2 d 2.22</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
<td>2 c 2.22</td>
<td>0,1/2,0 [0,0,0]</td>
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<td>1/2,0,0 [0,0,0]</td>
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</tr>
<tr>
<td>2 b 4'..</td>
<td>0,0,1/2 [0,0,0]</td>
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<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2 a 4'..</td>
<td>0,0,0 [0,0,0]</td>
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<tr>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
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</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1] p4g'm'  
\[ a^* = a, \quad b^* = b \]  
Origin at 0,0,z

Along [1,0,0] p1m'1  
\[ a^* = b/2, \quad b^* = c \]  
Origin at x,0,0

Along [1,1,0] p2m1'm'  
\[ a^* = (-a + b)/2, \quad b^* = c \]  
Origin at x,x,0
Origin on 4'12,'

Asymmetric unit
\[0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2\]

Symmetry Operations

\[
(1) \ 1 \\
(1') 0,0,0 \\
(2) \ 2 \ 0,0,z \\
(2') 0,0,0 \\
(3) \ 4' \ 0,0,z; 0,0,0 \\
(4) \ 4' \ 0,0,z; 0,0,0' \\
(5) \ a \ (1/2,0,0) \ x,1/4,z \\
(5') \ (1/2,1/2,0) \ (2y,1/2,0) \\
(6) \ b \ (0,1/2,0) \ 1/4,y,z \\
(6') \ (2x,1/2,1/2,0) \\
(7) \ 2' \ (1/2,1/2,0) \ x,x,0 \\
(7') \ (2x,1/2,1/2,0) \\
(8) \ 2' \ x,x+1/2,0 \\
(8') \ (2x,1/2,1/2,0)'
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
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<tr>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm  
Along [1,0,0] p2a1m1  
Along [1,1,0] p2mm'  
a* = a  b* = b  
a* = b/2  b* = c  
a* = -c  b* = (-a + b)/2  
Origin at 0,0,z  
Origin at x,1/4,0  
Origin at x,x,0
**Origin** on $\overline{4}1'2'_z$.

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

**Symmetry Operations**

1. $1$
   - $(1'0,0,0)$
   - $(m_y,1/2,1/2,0)'$

2. $2$ $0,0,z$
   - $(2_z,0,0,0)$
   - $(m_y,1/2,1/2,0)'$

3. $\overline{4}^+$ $0,0,z; 0,0,0$
   - $(4_z,0,0,0)$
   - $(4_z^{-1},0,0,0)$

4. $\overline{4}$ $0,0,z ; 0,0,0$
   - $(4_z,0,0,0)$
   - $(4_z^{-1},0,0,0)$

5. $a'$ $(1/2,2,0,0)$ $x,1/4,z$
   - $(m_x,1/2,1/2,0)'$

6. $b' (0,1/2,0)$ $1/4,y,z$
   - $(m_x,1/2,1/2,0)'$

7. $2' (1/2,1/2,0)$ $x,x,0$
   - $(2_{xy},1/2,1/2,0)'$

8. $2' x,x+1/2,0$
   - $(2_{xy},1/2,1/2,0)'$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Coordinates</th>
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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,z,v [v,u,w]</td>
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<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p4'g'm
a* = a  b* = b  c* = c
Origin at 0,0,0

Along [1,0,0] p1m'1
a* = b/2  b* = c  c* = c
Origin at x,0,0

Along [1,1,0] p2'mm'
a* = -c  b* = (-a + b)/2  c* = c
Origin at x,x,0

Origin at 0,0,z

117.5.962 - 2 - 1921
Origin on $\overline{4}12_1$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) + set$

(1) 1
(1) 0,0,0)

(5) a (1/2,0,0) x,1/4,z
(m, 1/2,1/2,0)

(6) b (0,1/2,0) 1/4,y,z
(m, 1/2,1/2,0)

(7) 2 (1/2,1/2,0) x,x,0
(2y, 1/2,1/2,0)

(8) 2' x,x+1/2,0
(2y, 1/2,1/2,0)

For $(0,0,1)' + set$

(1) t' (0,0,1)
(1) 0,0,1')

(5) n' (1/2,0,1) x,1/4,z
(m, 1/2,1/2,1')

(6) n' (0,1/2,1) 1/4,y,z
(m, 1/2,1/2,1')

(7) 2' (1/2,1/2,0) x,x,1/2
(2y, 1/2,1/2,1')

(8) 2' x,x+1/2,1/2
(2y, 1/2,1/2,1')

117.6.963 - 1 - 1922
Continued 117.6.963

Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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<td>(2) x,y,z [u,v,w]</td>
</tr>
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<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
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<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<tr>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
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</table>

| 8 h          | x,x+1/2,1/2 [u,u,w]                |
|              | x+1/2,x,1/2 [u,u,w]                |
|              | x+1/2,x,1/2 [u,u,w]                |
|              | x+1/2,x,1/2 [u,u,w]                |
| 8 g          | x,x+1/2,0 [u,u,0]                  |
|              | x+1/2,x,0 [u,u,0]                  |
|              | x+1/2,x,0 [u,u,0]                  |
| 8 f          | 0,1/2,z [0,0,w]                    |
|              | 1/2,0,z [0,0,w]                    |
|              | 1/2,0,z [0,0,w]                    |
| 8 e          | 0,0,z [0,0,w]                      |
|              | 0,0,z [0,0,w]                      |
|              | 1/2,1/2,z [0,0,w]                  |
|              | 1/2,1/2,z [0,0,w]                  |
| 4 d          | 0,1/2,1/2 [0,0,w]                  |
|              | 1/2,0,1/2 [0,0,w]                  |
| 4 c          | 0,1/2,0 [0,0,0]                    |
|              | 1/2,0,0 [0,0,0]                    |
| 4 b          | 0,0,1/2 [0,0,0]                    |
|              | 1/2,1/2,1/2 [0,0,0]                |
| 4 a          | 0,0,0 [0,0,w]                      |
|              | 1/2,1/2,0 [0,0,w]                  |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4gm1'</th>
<th>Along [1,0,0]</th>
<th>p_{2c}1m1</th>
<th>Along [1,1,0]</th>
<th>p_{2c}2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
<td>a^* = b/2</td>
<td>b^* = c</td>
<td>a^* = -c</td>
<td>b^* = (-a + b)/2</td>
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</tbody>
</table>

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at x,x,0
P2₁\bar{4}b'2

\begin{align*}
\text{Asymmetric unit} &: 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2 \\
\text{Symmetry Operations} &
\begin{align*}
&\begin{array}{l}
(1) 1 \\
(5) a' (1/2,0,0) \quad x,1/4,z \\
\end{array} \\
&\begin{array}{l}
(2) 2' (0,0,1) \quad 0,0,z \\
(6) b' (1/2,1/2,0) \quad 1/4,y,z \\
\end{array} \\
&\begin{array}{l}
(3) \bar{4}^{-} \quad 0,0,z; 0,0,0 \\
(7) 2' (1/2,1/2,0) \quad x,x,1/2 \\
\end{array} \\
&\begin{array}{l}
(4) \bar{4}^{-} \quad 0,0,z; 0,0,0 \\
(8) x,x+1/2,0 \\
\end{array} \\
\end{align*}
\end{align*}
Continued

Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5).

Positions

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<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<tbody>
<tr>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) y+1/2,x+1/2,z [v,u,w]</td>
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</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z [v,u,w]</td>
<td></td>
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</tbody>
</table>

| 8 h ..2'     | x,x+1/2,1/2 [u,u,w] |
|              | x,x+1/2,1/2 [u,u,w] |
|              | x+1/2,x,1/2 [u,u,w] |
|              | x+1/2,x,1/2 [u,u,w] |

| 8 g ..2      | x,x+1/2,0 [u,u,0] |
|              | x,x+1/2,0 [u,u,0] |
|              | x+1/2,x,0 [u,u,0] |
|              | x+1/2,x,0 [u,u,0] |

| 8 f 2..      | 0,1/2,z [0,0,w] |
|              | 1/2,0,z [0,0,w] |
|              | 1/2,0,z [0,0,w] |
|              | 0,1/2,z [0,0,w] |

| 8 e 2..      | 0,0,z [0,0,w] |
|              | 0,0,z [0,0,w] |
|              | 1/2,1/2,z [0,0,w] |
|              | 1/2,1/2,z [0,0,w] |

| 4 d 2.2'2'   | 0,1/2,1/2 [0,0,w] |
|              | 1/2,0,1/2 [0,0,w] |

| 4 c 2.22     | 0,1/2,0 [0,0,0] |
|              | 1/2,0,0 [0,0,0] |

| 4 b 4..      | 0,0,1/2 [0,0,w] |
|              | 1/2,1/2,1/2 [0,0,w] |

| 4 a 4'..     | 0,0,0 [0,0,0] |
|              | 1/2,1/2,0 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4gm1'  Along [1,0,0] p2a'1m1'  Along [1,1,0] p2a'2m'm'

a* = a  b* = b  a* = a/2  b* = c  a* = -c  b* = (-a + b)/2

Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0

117.7.964 - 2 - 1925
Origin on $\bar{4}$

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/4$

Symmetry Operations

(1) $1$

(1) $0,0,0$

(5) $n (1/2,0,1/2) \ x,1/4,z$

(6) $n (0,1/2,1/2) \ 1/4,y,z$

(7) $2 (1/2,1/2,0) \ x,x,1/4$

(8) $2 \ x,x+1/2,1/4$

(2) $2 \ 0,0,z$

(2) $0,0,0$

(3) $\bar{4}^+ \ 0,0,z; 0,0,0$

(3) $\bar{4}^+ \ 0,0,0$

(4) $\bar{4} \ 0,0,z; 0,0,0$

(4) $\bar{4} \ 0,0,0$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

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<td>8 i 1</td>
<td>x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td>(3) y,x,z</td>
<td>[v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
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<tr>
<td>(5) x+1/2, y+1/2, z+1/2</td>
<td>[u,v,w]</td>
<td>(6) x+1/2, y+1/2, z+1/2</td>
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<tr>
<td>(7) y+1/2, x+1/2, z+1/2</td>
<td>[v,u,w]</td>
<td>(8) y+1/2, x+1/2, z+1/2</td>
</tr>
</tbody>
</table>

| 4 h 2         | 0,1/2,0, [0,0,0] | 1/2,0,0, z [0,0,w] |
| 4 g .2        | x,x+1/2,1/4, [u,u,0] | x+1/2, x,3/4, [u,u,0] |
| 4 f .2        | x,x+1/2,1/4, [u,u,0] | x+1/2, x,3/4, [u,u,0] |
| 4 e 2         | 0,0,0, [0,0,0] | 0,0,0, [0,0,0] |
| 2 d 2.22      | 0,1/2,3/4, [0,0,0] | 1/2,0,1/4, [0,0,0] |
| 2 c 2.22      | 0,1/2,1/4, [0,0,0] | 1/2,0,3/4, [0,0,0] |
| 2 b .4        | 0,0,1/2, [0,0,0] | 1/2,1/2,0, [0,0,0] |
| 2 a .4        | 0,0,0, [0,0,0] | 1/2,1/2,1/2, [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4'gm'  Along [1,0,0] c_p,1m1'  Along [1,1,0] p2m1m1'

a^* = a  b^* = b  a^* = b  b^* = c  a^* = (-a + b)/2  b^* = c

Origin at 0,0,z  Origin at x,0,0  Origin at x,x,1/4
Origin on $\overline{4}1'$

Asymmetric unit
$0 \leq x \leq 1/2$; $0 \leq y \leq 1$; $0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

(1) 1
(1) 0,0,0

(5) n (1/2,0,1/2) $x,1/4,z$
($m_{y}|1/2,1/2,1/2$)

(6) n (0,1/2,1/2) $1/4,y,z$
($m_{x}|1/2,1/2,1/2$)

(7) 2 (1/2,1/2,0) $x,x,1/4$
($2_{xy}|1/2,1/2,1/2$)

For 1' + set

(1) 1'
(1) 0,0,0'$

(5) n' (1/2,0,1/2) $x,1/4,z$
($m_{y}|1/2,1/2,1/2'$)

(6) n' (0,1/2,1/2) $1/4,y,z$
($m_{x}|1/2,1/2,1/2'$)

(7) 2' (1/2,1/2,0) $x,x,1/4$
($2_{xy}|1/2,1/2,1/2'$)

(8) 2' $x,x+1/2,1/4$
($2_{xy}|1/2,1/2,1/2'$)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); 1'.

Positions

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<td>(2) x,y,z [0,0,0]</td>
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<td>(4) y,x,z [0,0,0]</td>
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<td>(5) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
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<td>(6) x+1/2,y+1/2,z+1/2 [0,0,0]</td>
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<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
<td></td>
<td>(8) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 h 2.1'</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
<td>1/2,0,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 g .21'</td>
<td>x+1/2,1/4 [0,0,0]</td>
<td>x+1/2,1/4 [0,0,0]</td>
<td>x+1/2,x+1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 f .21'</td>
<td>x+1/2,1/4 [0,0,0]</td>
<td>x+1/2,1/4 [0,0,0]</td>
<td>x+1/2,x+1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 e 2.1'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 d 2.221'</td>
<td>0,1/2,3/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 c 2.221'</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,0,3/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b 4.1'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 4.1'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1'  Along [1,0,0] c1m11'  Along [1,1,0] p2mm1'

\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \quad \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \quad \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \)

Origin at 0,0,z  Origin at x,0,0  Origin at x,x,1/4
Origin on \( \overline{4} \cdot \nabla \).

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

(1) \( 1 \\
(1) \quad 0,0,0 \)

(2) \( 2 \quad 0,0,z \)

(3) \( \overline{4} \cdot \nabla \quad 0,0,z; 0,0,0 \)

(4) \( \overline{4} \cdot \nabla \quad 0,0,z; 0,0,0 \)

(5) \( n'(1/2,0,1/2) \quad x,1/4,z \)

(6) \( n'(0,1/2,1/2) \quad 1/4,y,z \)

(7) \( 2 \quad (1/2,1/2,0) \quad x,x,1/4 \)

(8) \( 2 \quad x,x+1/2,1/4 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)

\( \overline{4}' \cdot \nabla' \quad 0,0,0 \)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4g'm'</th>
<th>Along [1,0,0]</th>
<th>c1m'1</th>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,x,1/4</td>
<td></td>
</tr>
</tbody>
</table>
Origin on \( \overline{4} \cdot \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

\begin{align*}
(1) \quad & 1 \\
(1') \quad & 0,0,0 \\
(2) \quad & 0,0,z \\
(2z) \quad & 0,0,0 \\
(3) \quad & \overline{4} \cdot , \quad 0,0,z; \quad 0,0,0 \\
(4) \quad & \overline{4} \cdot \quad 0,0,z; \quad 0,0,0 \\
(5) \quad & n \quad (1/2,0,1/2) \\
(5') \quad & x,1/4,z \\
(6) \quad & n \quad (0,1/2,1/2) \\
(6') \quad & 1/4,y,z \\
(7) \quad & 2' \quad (1/2,1,2/0) \\
(7') \quad & x,x,1/4 \\
(8) \quad & 2' \quad x,x+1/2,1/4 \\
(8') \quad & 2'y,1/2,1/2' \\
\end{align*}
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

---

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2, x+1/2, z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y+1/2, x+1/2, z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

---

**Symmetry of Special Projections**

- **Along [0,0,1]**: p4gm
  - **a** = a
  - **b** = b
  - Origin at 0,0,z

- **Along [1,0,0]**: c_,1m'1
  - **a** = b
  - **b** = c
  - Origin at x,0,0

- **Along [1,1,0]**: p2'mm'
  - **a** = -c
  - **b** = (-a + b)/2
  - Origin at x,x,1/4

---
Origin on \( \bar{4} \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

1. \( 1 \)
   \( (1) \quad 1 \)
   \( (2) \quad 2, 0,0,0 \)
   \( (3) \quad \bar{4}, 0,0,0; 0,0,0 \)
   \( (4) \quad \bar{4}, 0,0,0; 0,0,0 \)

2. \( n' \)
   \( (5) \quad (1/2,0,1/2), x,1/4,z \)
   \( (6) \quad (0,1/2,1/2), 1/4,y,z \)
   \( (7) \quad 2', (1/2,1/2,0), x,x,1/4 \)
   \( (8) \quad 2', x,x+1/2,1/4 \)

3. \( \bar{4}n'2' \)
   \( \bar{4}m'2' \)

4. \( \bar{4}n'2' \)

5. Tetragonal

6. 118.5.969

7. 118.5.969 - 1 - 1934
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w] (6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w] (8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

4 h 2.. 0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 0,1/2,z+1/2 [0,0,w]

4 g ..2' x,x+1/2,1/4 [u,u,w] x+1/2,x,3/4 [u,u,w] x+1/2,x,3/4 [u,u,w]

4 f ..2' x,x+1/2,1/4 [u,u,w] x+1/2,x,3/4 [u,u,w] x+1/2,x,3/4 [u,u,w]

4 e 2.. 0,0,z [0,0,w] 0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w]

2 d 2.2' 0,1/2,3/4 [0,0,w] 1/2,0,1/4 [0,0,w]

2 c 2.2' 0,1/2,1/4 [0,0,w] 1/2,0,3/4 [0,0,w]

2 b 4.. 0,0,1/2 [0,0,w] 1/2,1/2,0 [0,0,w]

2 a 4.. 0,0,0 [0,0,w] 1/2,1/2,1/2 [0,0,w]

Symmetry of Special Projections

Along [1,0,0] p4'g'm Along [1,1,0] p2mm'

a* = a  b* = b  a* = -c  b* = (-a + b)/2

Origin at 0,0,z Origin at x,0,0 Origin at x,x,1/4
$P_{4\bar{n}2}$

$118.6.970$

$\bar{4}m21'$

Tetragonal

$P_{4\bar{n}2}$

$118.6.970 - 1 - 1936$
**Origin** on $\overline{4}$

**Asymmetric unit**  $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

For $(0,0,0)$ + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td>(2) 2</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(3) $\overline{4}$</td>
<td>$0,0,z; 0,0,0$</td>
</tr>
<tr>
<td>(4) $\overline{4}$</td>
<td>$0,0,0; 0,0,0$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5) $n$</td>
<td>$1/2,0,1/2; \quad y,1/4,z$</td>
</tr>
<tr>
<td>(6) $n$</td>
<td>$1/2,1/2,0; \quad y,x,1/4$</td>
</tr>
<tr>
<td>(7) $2$</td>
<td>$1/2,1/2,0; \quad x,x,1/4$</td>
</tr>
<tr>
<td>(8) $2$</td>
<td>$1/2,1/2,0; \quad x,x,1/4$</td>
</tr>
</tbody>
</table>

For $(1,0,0)'$ + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $t'$</td>
<td>$(1,0,0)$</td>
</tr>
<tr>
<td>(2) $2'$</td>
<td>$1/2,0,z$</td>
</tr>
<tr>
<td>(3) $\overline{4}'$</td>
<td>$1/2,1/2,0; \quad 1/2,1/2,0$</td>
</tr>
<tr>
<td>(4) $\overline{4}'$</td>
<td>$1/2,1/2,0; \quad 1/2,1/2,0$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5) $n'$</td>
<td>$3/2,0,1/2; \quad y,x,1/4$</td>
</tr>
<tr>
<td>(6) $n'$</td>
<td>$3/2,1/2,0; \quad y,x,1/4$</td>
</tr>
<tr>
<td>(7) $2'$</td>
<td>$3/2,1/2,0; \quad x,x,1/4$</td>
</tr>
<tr>
<td>(8) $2'$</td>
<td>$3/2,1/2,0; \quad x,x,1/4$</td>
</tr>
</tbody>
</table>

**Generators selected**  $(1); \quad t'(1,0,0); \quad t'(0,1,0); \quad t'(0,0,1); \quad (2); \quad (3); \quad (5)$.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>$16$  $i$  $1$</td>
<td></td>
</tr>
<tr>
<td>$16$  $i$  $1$</td>
<td></td>
</tr>
<tr>
<td>$16$  $i$  $1$</td>
<td></td>
</tr>
<tr>
<td>$16$  $i$  $1$</td>
<td></td>
</tr>
<tr>
<td>$8$   $h$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$8$   $g$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$8$   $f$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$8$   $e$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $d$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $c$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $b$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $a$  $2'$</td>
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</tbody>
</table>

<table>
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<tr>
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<td>(1,0,0)' +</td>
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<tr>
<td>$16$  $i$  $1$</td>
<td></td>
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<td>$16$  $i$  $1$</td>
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<tr>
<td>$8$   $h$  $2'$</td>
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<tr>
<td>$8$   $g$  $2'$</td>
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</tr>
<tr>
<td>$8$   $f$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$8$   $e$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $d$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $c$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $b$  $2'$</td>
<td></td>
</tr>
<tr>
<td>$4$   $a$  $2'$</td>
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</tbody>
</table>
## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4gm1'</td>
<td>$a^* = a$, $b^* = b$</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>c1m11'</td>
<td>$a^* = b$, $b^* = c$</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p c* 2mm</td>
<td>$a^* = (-a + b)/2$, $b^* = c$</td>
</tr>
</tbody>
</table>
**Origin on 4m2**

**Asymmetric unit**

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/4 \]

**Symmetry Operations**

**For (0,0,0) + set**

1. \( 1 \)
2. \( 2 \) \( 0,0,z \) \( (2_z 0,0,0) \)
3. \( \bar{4} \) \( 0,0,z; 0,0,0 \) \( (4_z 0,0,0) \)
4. \( 4 \) \( 0,0,z; 0,0,0 \) \( (4_z 0,0,0) \)
5. \( m \) \( x,0,z \) \( (m_x 0,0,0) \)
6. \( m \) \( y,z \) \( (m_y 0,0,0) \)
7. \( 2 \) \( x,x,0 \) \( (2_{xy} 0,0,0) \)
8. \( 2 \) \( x,x,0 \) \( (2_{xy} 0,0,0) \)

**For (1/2,1/2,1/2) + set**

1. \( t \) \( 1/2,1/2,1/2 \)
2. \( 2 \) \( 0,0,1/2 \) \( 1/4,1/4,z \) \( (2_z 1/2,1/2,1/2) \)
3. \( \bar{4} \) \( 1/2,0,z; 1/2,0,1/4 \) \( (4_z 1/2,1/2,1/2) \)
4. \( 4 \) \( 0,1/2,2,1/2 \)
5. \( n \) \( 1/2,0,1/2 \) \( x,1/4,z \) \( (m_y 1/2,1/2,1/2) \)
6. \( n \) \( 0,1/2,1/2 \) \( 1/4,y,z \) \( (m_x 1/2,1/2,1/2) \)
7. \( 2 \) \( 1/2,1/2,0 \) \( x,x,1/4 \) \( (2_{xy} 1/2,1/2,1/2) \)
8. \( 2 \) \( x,x+1/2,1/4 \) \( (2_{xy} 1/2,1/2,1/2) \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 i .m.</td>
<td>(5) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>8 h .2</td>
<td>(x, x, 0) [u, u, 0]</td>
</tr>
<tr>
<td>4 f 2mm.</td>
<td>0, 1/2, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>4 e 2mm.</td>
<td>0, 0, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>2 d 4m2</td>
<td>0, 1/2, 3/4 [0, 0, 0]</td>
</tr>
<tr>
<td>2 c 4m2</td>
<td>0, 1/2, 1/4 [0, 0, 0]</td>
</tr>
<tr>
<td>2 b 4m2</td>
<td>0, 0, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>2 a 4m2</td>
<td>0, 0, 0 [0, 0, 0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'm'm
\[ a^* = (a - b)/2 \] \[ b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] c1m11'
\[ a^* = b \] \[ b^* = c \]
Origin at 0,0,0

Along [1,1,0] p2m'm'
\[ a^* = (-a + b)/2 \] \[ b^* = c/2 \]
Origin at x,0,0
I4 m2\textsuperscript{1}'

119.2.972

\begin{align*}
\overline{4}m2\textsuperscript{1}' & \quad \text{Tetragonal} \\
\end{align*}

\begin{align*}
\text{Origin} & \quad \text{on} \; \overline{4}m2\textsuperscript{1}' \\
\text{Asymmetric unit} & \quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \\
\text{Symmetry Operations} & \\
\text{For} \; (0,0,0) \; \text{+ set} & \\
(1) & \; 1 \\
(2) & \; 2 \; 0,0,0 \quad (2\bar{z} \; 0,0,0) \\
(3) & \; \overline{4} \; 0,0,z; 0,0,0 \quad (4\bar{z} \; 0,0,0) \\
(4) & \; \overline{4} \; 0,0,z; 0,0,0 \quad (4\bar{z} \; 0,0,0) \\
(5) & \; m \; x,0,z \quad (m_x \; 0,0,0) \\
(6) & \; m \; 0,y,z \quad (m_y \; 0,0,0) \\
(7) & \; 2 \; x,y,0 \quad (2z_x \; 0,0,0) \\
(8) & \; 2 \; x,y,0 \quad (2z_y \; 0,0,0) \\
\text{For} \; (1/2,1/2,1/2) \; \text{+ set} & \\
(1) & \; t \; (1/2,1/2,1/2) \\
(2) & \; 2 \; (0,0,1/2) \quad 1/4,1/4,z \quad (2\bar{z} \; 1/2,1/2,1/2) \\
(3) & \; \overline{4} \; 1/2,0,z; 1/2,0,1/4 \\
(4) & \; \overline{4} \; 0,1/2,z; 0,1/2,1/4 \quad (4\bar{z} \; 1/2,1/2,1/2) \\
(5) & \; n \; (1/2,0,1/2) \; x,1/4,z \\
(6) & \; n \; (0,1/2,1/2) \; 1/4,y,z \\
(7) & \; 2 \; (1/2,1/2,0) \; x,x,1/4 \\
(8) & \; 2 \; x,x+1/2,1/4 \\
\end{align*}
Continued 119.2.972  

For (0,0,0) + set

(1) 1'  
  (1) 0,0,0'  
(2) 2' 0,0,z  
  (2) z,0,0',0  
(3) 4' 0,0,z; 0,0,0  
  (4) 4' 0,0,z; 0,0,0  
(5) m' x,0,z  
  (m) x,0,0,0'  
(6) m' 0,y,z  
  (m) 0,0,0',0  
(7) 2' x,x,0  
  (2,2) 0,0,0'  
(8) 2' x,x,0  
  (2,2) 0,0,0'

For (1/2,1/2,1/2) + set

(1) t' (1/2,1/2,1/2)  
  (1) 1/2,1/2,1/2'  
(2) 2' (0,0,1/2)  
  (2) z,1/2,1/2,1/2'  
(3) 4' 1/2,0,z; 1/2,0,1/4  
  (4) 4' 1/2,0,z; 1/2,0,1/4  
(5) n' (1/2,0,1/2)  
  (m) 1/2,1/2,1/2'  
(6) n' (0,1/2,1/2)  
  (m) 1/2,1/2,1/2'  
(7) 2' (1/2,1/2,0)  
  (2,2) 1/2,1/2,1/2'  
(8) 2' (1/2,1/2,1/2)  
  (2,2) 1/2,1/2,1/2'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5): 1'.

Positions

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>(0,0,0) +</th>
<th>(1/2,1/2,1/2) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 j 11' x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
<td>(3) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>8 i .m.1' x,0,z [0,0,0]</td>
<td>(5) x,0,z [0,0,0]</td>
<td>(6) x,0,z [0,0,0]</td>
</tr>
<tr>
<td>8 h .21' x,x+1/2,1/4 [0,0,0]</td>
<td>(9) x,x+1/2,1/4 [0,0,0]</td>
<td>(10) x,x+1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4 f 2mm.1' 0,1/2,z [0,0,0]</td>
<td>(12) 0,1/2,z [0,0,0]</td>
<td>(13) 0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 e 2mm.1' 0,0,z [0,0,0]</td>
<td>(15) 0,0,z [0,0,0]</td>
<td>(16) 0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d 4m21' 0,1/2,3/4 [0,0,0]</td>
<td>(18) 0,1/2,3/4 [0,0,0]</td>
<td>(19) 0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 c 4m21' 0,1/2,1/4 [0,0,0]</td>
<td>(21) 0,1/2,1/4 [0,0,0]</td>
<td>(22) 0,1/2,1/4 [0,0,0]</td>
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<tr>
<td>2 b 4m21' 0,0,1/2 [0,0,0]</td>
<td>(24) 0,0,1/2 [0,0,0]</td>
<td>(25) 0,0,1/2 [0,0,0]</td>
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<tr>
<td>2 a 4m21' 0,0,0 [0,0,0]</td>
<td>(27) 0,0,0 [0,0,0]</td>
<td>(28) 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1'</th>
<th>Along [1,0,0] c1m11'</th>
<th>Along [1,1,0] p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = (a - b)/2  b' = (a + b)/2</td>
<td>a' = b  b' = c</td>
<td>a' = -(a + b)/2  b' = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

119.2.972 - 2 - 1942
I$\bar{4}$m'2

119.3.973

I$\bar{4}$m'2

Tetragonal

Origin on $\bar{4}$m'2

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For (0,0,0) + set

1. 1

(1) 1

(1) 0,0,0

(5) m' x,0,z

(5) m' (0,0,0)

(5) (m,0,0,0')

2. 2 0,0,z

(2) 0,0,0

(6) m' 0,y,z

(6) m' (0,0,0)

(6) (m,0,0,0')

$2z\downarrow\rightarrow 0,0,0$

$2x\downarrow\rightarrow 0,0,0$

$2y\downarrow\rightarrow 0,0,0$

$4z\downarrow\rightarrow 0,0,0$

$4x\downarrow\rightarrow 0,0,0$

$4y\downarrow\rightarrow 0,0,0$

$4\downarrow\rightarrow 0,0,0$

$4\downarrow\rightarrow 0,0,0$

3. $\bar{4}$m' 0,0,z; 0,0,0

(3) $\bar{4}$m' 0,0,0;

(3) 0,0,0

(7) 2 x,x,0

(7) 2 (0,0,0)

$2x\downarrow\rightarrow 0,0,0$

$2y\downarrow\rightarrow 0,0,0$

$2z\downarrow\rightarrow 0,0,0$

$4z\downarrow\rightarrow 0,0,0$

$4x\downarrow\rightarrow 0,0,0$

$4y\downarrow\rightarrow 0,0,0$

$4\downarrow\rightarrow 0,0,0$

4. $\bar{4}$m' 0,0,z; 0,0,0

(4) $\bar{4}$m' 0,0,0;

(4) 0,0,0

(8) 2 x,x,0

(8) 2 (0,0,0)

$2x\downarrow\rightarrow 0,0,0$

$2y\downarrow\rightarrow 0,0,0$

$2z\downarrow\rightarrow 0,0,0$

$4z\downarrow\rightarrow 0,0,0$

$4x\downarrow\rightarrow 0,0,0$

$4y\downarrow\rightarrow 0,0,0$

$4\downarrow\rightarrow 0,0,0$

For (1/2,1/2,1/2) + set

1. t (1/2,1/2,1/2)

(1) t (1/2,1/2,1/2)

(1) 0,0,1/2

(1) 0,0,1/2

(1) 0,0,1/2

2. 2 (0,0,1/2) 1/4,1/4,z

(2) (0,0,1/2)

(2) 1/4,1/4,z

(2) 1/4,1/4,z

$2z\downarrow\rightarrow 1/2,1/2,1/2$

$2x\downarrow\rightarrow 1/2,1/2,1/2$

$2y\downarrow\rightarrow 1/2,1/2,1/2$

$4z\downarrow\rightarrow 1/4,1/4,1/4$

$4x\downarrow\rightarrow 1/4,1/4,1/4$

$4y\downarrow\rightarrow 1/4,1/4,1/4$

3. $\bar{4}$m' 1/2,0,z; 1/2,0,1/4

(3) $\bar{4}$m' 1/2,0,0;

(3) 1/2,0,1/4

(3) 1/2,0,1/4

$2z\downarrow\rightarrow 1/2,1/2,1/2$

$2x\downarrow\rightarrow 1/2,1/2,1/2$

$2y\downarrow\rightarrow 1/2,1/2,1/2$

$4z\downarrow\rightarrow 1/2,1/2,1/2$

$4x\downarrow\rightarrow 1/2,1/2,1/2$

$4y\downarrow\rightarrow 1/2,1/2,1/2$

4. $\bar{4}$m' 0,1/2,z; 0,1/2,1/4

(4) $\bar{4}$m' 0,1/2,0;

(4) 0,1/2,1/4

(4) 0,1/2,1/4

$2z\downarrow\rightarrow 1/2,1/2,1/2$

$2x\downarrow\rightarrow 1/2,1/2,1/2$

$2y\downarrow\rightarrow 1/2,1/2,1/2$

$4z\downarrow\rightarrow 1/2,1/2,1/2$

$4x\downarrow\rightarrow 1/2,1/2,1/2$

$4y\downarrow\rightarrow 1/2,1/2,1/2$

5. n' (1/2,0,1/2) x,1/4,z

(5) n' (1/2,0,1/2)

(5) x,1/4,z

(5) x,1/4,z

$2z\downarrow\rightarrow 1/4,1/4,1/4$

$2x\downarrow\rightarrow 1/4,1/4,1/4$

$2y\downarrow\rightarrow 1/4,1/4,1/4$

$4z\downarrow\rightarrow 1/4,1/4,1/4$

$4x\downarrow\rightarrow 1/4,1/4,1/4$

$4y\downarrow\rightarrow 1/4,1/4,1/4$

6. n' (0,1/2,1/2) 1/4,y,z

(6) n' (0,1/2,1/2)

(6) 1/4,y,z

(6) 1/4,y,z

$2z\downarrow\rightarrow 1/4,1/4,1/4$

$2x\downarrow\rightarrow 1/4,1/4,1/4$

$2y\downarrow\rightarrow 1/4,1/4,1/4$

$4z\downarrow\rightarrow 1/4,1/4,1/4$

$4x\downarrow\rightarrow 1/4,1/4,1/4$

$4y\downarrow\rightarrow 1/4,1/4,1/4$

7. 2 (1/2,1/2,0) x,x,1/4

(7) 2 (1/2,1/2,0)

(7) x,x,1/4

(7) x,x,1/4

$2x\downarrow\rightarrow 1/2,1/2,1/2$

$2y\downarrow\rightarrow 1/2,1/2,1/2$

$2z\downarrow\rightarrow 1/2,1/2,1/2$

$4x\downarrow\rightarrow 1/2,1/2,1/2$

$4y\downarrow\rightarrow 1/2,1/2,1/2$

$4z\downarrow\rightarrow 1/2,1/2,1/2$

8. 2 x,x+1/2,1/4

(8) 2 (x,x+1/2,1/4)

(8) x,x+1/2,1/4

(8) x,x+1/2,1/4

$2x\downarrow\rightarrow 1/2,1/2,1/2$

$2y\downarrow\rightarrow 1/2,1/2,1/2$

$2z\downarrow\rightarrow 1/2,1/2,1/2$
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

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### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>j</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td></td>
<td>(3) x,y,z [v,u,w]</td>
</tr>
<tr>
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<td>(4) x,y,z [v,u,w]</td>
</tr>
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<td>(5) x,y,z [u,v,w]</td>
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<tr>
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<td>(6) x,y,z [v,u,w]</td>
</tr>
<tr>
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<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) x,y,z [v,u,w]</td>
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</tbody>
</table>

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### Coordinates

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Generator</th>
</tr>
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<tbody>
<tr>
<td>16</td>
<td>x,y,z</td>
</tr>
<tr>
<td>8</td>
<td>u,v,w</td>
</tr>
<tr>
<td>8</td>
<td>u,v,w</td>
</tr>
<tr>
<td>8</td>
<td>u,v,w</td>
</tr>
<tr>
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<td>4</td>
<td>u,v,w</td>
</tr>
<tr>
<td>2</td>
<td>u,v,w</td>
</tr>
<tr>
<td>2</td>
<td>u,v,w</td>
</tr>
<tr>
<td>2</td>
<td>u,v,w</td>
</tr>
<tr>
<td>2</td>
<td>u,v,w</td>
</tr>
</tbody>
</table>

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### Symmetry of Special Projections

Along [0,0,1] p4m'2' Along [1,0,0] c1m'1

\[ a^* = \frac{a - b}{2} \quad b^* = \frac{a + b}{2} \]

Origin at 0,0,z

Along [1,1,0] p2m'1

\[ a^* = \frac{a + b}{2} \quad b^* = c/2 \]

Origin at x,x,0
Origin on $\overline{4}m2'$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

**For (0,0,0) + set**

1. $I = (0,0,0)$
2. $2 \cdot 0,0,z \quad (2z \cdot 0,0,0)$
3. $4 \cdot 0,0,z; 0,0,0 \quad (4z \cdot 0,0,0)'$
4. $4 \cdot 0,0,z; 0,0,0 \quad (4z^{-1} \cdot 0,0,0)'$

5. $m \cdot x,0,z \quad (m \cdot x,0,0,0)$
6. $m \cdot 0,y,z \quad (m \cdot 0,y,0,0)$
7. $2' \cdot x,x,0 \quad (2'xy \cdot 0,0,0)'$
8. $2' \cdot x,x,0 \quad (2'xy \cdot 0,0,0)'$

**For (1/2,1/2,1/2) + set**

1. $t \cdot (1/2,1/2,1/2)$
2. $2 \cdot (0,0,1/2) \quad 1/4,1/4,z \quad (2z \cdot 1/2,1/2,1/2)$
3. $4 \cdot 1/2,0,z; 1/2,0,1/4 \quad (4z \cdot 1/2,1/2,1/2)'$
4. $4 \cdot 0,1/2,z; 0,1/2,1/4 \quad (4z^{-1} \cdot 1/2,1/2,1/2)'$

5. $n \cdot (1/2,0,1/2) \quad x,1/4,z \quad (m \cdot 1/2,1/2,1/2)$
6. $n \cdot (0,1/2,1/2) \quad 1/4,y,z \quad (m \cdot 1/2,1/2,1/2)$
7. $2' \cdot (1/2,1/2,0) \quad x,x,1/4 \quad (2'xy \cdot 1/2,1/2,1/2)'$
8. $2' \cdot x,x,1/2,1/4 \quad (2'xy \cdot 1/2,1/2,1/2)'$

119.4.974 - 1 - 1945
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
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<tr>
<td>16 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<td></td>
<td>(2) (\bar{x},y,z) [u,v,w]</td>
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<td></td>
<td>(3) (x,\bar{x},z) [v,u,w]</td>
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<td>(4) (y,\bar{x},z) [v,u,w]</td>
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<td>(5) (x,\bar{y},z) [u,v,w]</td>
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<td>(7) (y,x,z) [v,u,w]</td>
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<td>(8) (\bar{y},x,z) [v,u,w]</td>
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<tr>
<td>8 i .m.</td>
<td>x,0,z [0,v,0]</td>
<td>0,x,(\bar{z}) [v,0,0]</td>
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<td>(\bar{x},0,z) [0,v,0]</td>
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<tr>
<td>8 h .2'</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
<td>(\bar{x}+1/2,x,3/4) [u,u,w]</td>
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<td></td>
<td>(x,x+1/2,1/4) [u,u,w]</td>
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<td>(x+1/2,x,3/4) [u,u,w]</td>
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<td>8 g .2'</td>
<td>x,x,0 [u,u,w]</td>
<td>(x,x,0) [u,u,w]</td>
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<td>(\bar{x},\bar{x},0) [u,u,w]</td>
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<td>(x,\bar{x},0) [u,u,w]</td>
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<tr>
<td>4 f 2mm.</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,(\bar{z}) [0,0,0]</td>
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<tr>
<td>4 e 2mm.</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,(\bar{z}) [0,0,0]</td>
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<tr>
<td>2 d (\bar{4})m2'</td>
<td>0,1/2,3/4 [0,0,0]</td>
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<tr>
<td>2 c (\bar{4})m2'</td>
<td>0,1/2,1/4 [0,0,0]</td>
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<tr>
<td>2 b (\bar{4})m2'</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2 a (\bar{4})m2'</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm
\(a^* = (a - b)/2\) \(b^* = (a + b)/2\)
Origin at 0,0,z

Along [1,0,0] c1m11'
\(a^* = b\) \(b^* = c\)
Origin at x,0,0

Along [1,1,0] p2'mm'
\(a^* = -c/2\) \(b^* = (-a + b)/2\)
Origin at x,x,0
Origin on $\bar{4}m'2'$

Asymmetric unit  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0) +$ set:

1. $1$
  
2. $2 \quad 0,0,z$
   
3. $\bar{4} \quad 0,0,0; 0,0,0$
   
4. $\bar{4} \quad 0,0,0; 0,0,0$

For $(1/2,1/2,1/2) +$ set:

1. $t \quad (1/2,1/2,1/2)$

2. $2 \quad (0,0,1/2) \quad 1/4,1/4,z$
   
3. $\bar{4} \quad 1/2,1/2,1/2; 1/2,1/2,1/2$

4. $\bar{4} \quad 1/2,1/2,1/2; 1/2,1/2,1/2$

5. $n' \quad (1/2,0,1/2) \quad x,1/4,z$
   
6. $n' \quad (0,1/2,1/2) \quad 1/4,y,z$
   
7. $2' \quad (1/2,1/2,0) \quad x,x,1/4$

8. $2' \quad x,x+1/2,1/4$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Generators</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 j 1</td>
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<td>(1/2,1/2,1/2) +</td>
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<td>0,x,z [0,0,w]</td>
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<td>x,0,z [u,0,w]</td>
<td>0,x,z [0,0,w]</td>
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<td>8 h ..2'</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
<td>x+1/2,x,3/4 [u,u,w]</td>
</tr>
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<td>x+1/2,x,3/4 [u,u,w]</td>
</tr>
<tr>
<td>8 g ..2'</td>
<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
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<td>x,x,0 [u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td>4 f 2m'm'</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 2m'm'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<tr>
<td>2 d 4m2'</td>
<td>0,1/2,3/4 [0,0,w]</td>
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<td>2 c 4m2'</td>
<td>0,1/2,1/4 [0,0,w]</td>
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<tr>
<td>2 b 4m2'</td>
<td>0,0,1/2 [0,0,w]</td>
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</tr>
<tr>
<td>2 a 4m2'</td>
<td>0,0,0 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p4mm'; a' = (b - a)/2, b' = (a + b)/2
- Along [1,0,0] c1m'; a' = b, b' = c
- Along [1,1,0] p2mm'; a' = -c/2, b' = (-a + b)/2
- Origin at 0,0,z
- Origin at x,0,0
- Origin at x,x,0
**Origin** on $\bar{4}m2$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

For $(0,0,0) + \text{set}$

1. $1$

(1) $1$

(2) $2 \cdot 0,0,z$

(3) $\bar{4}^{-} \cdot 0,0,0$

(4) $\bar{4}^{-} \cdot 0,0,0$

For $(1/2,1/2,1/2)' + \text{set}$

(5) $m \cdot x,0,z$

(6) $m \cdot 0,y,z$

(7) $2 \cdot x,x,0$

(8) $2 \cdot x,x,0$

For $(1/2,1/2,1/2)' + \text{set}$

(1) $t' \cdot (1/2,1/2,1/2)$

(2) $2' \cdot (0,0,1/2)$

(3) $\bar{4}^{-}' \cdot 1/2,0,0$

(4) $\bar{4}^{-}' \cdot 0,1/2,0$

(5) $n' \cdot (1/2,0,1/2)$

(6) $n' \cdot (0,1/2,1/2)$

(7) $2' \cdot (1/2,1/2,0)$

(8) $2' \cdot x,0$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<th>Multiplicity</th>
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<tr>
<td>Wyckoff letter</td>
<td>j</td>
<td>i</td>
<td>h</td>
<td>g</td>
<td>f</td>
<td>e</td>
<td>d</td>
<td>c</td>
</tr>
<tr>
<td>Site Symmetry</td>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2)’ +</td>
<td>(0,0,0)</td>
<td>(0,v,0)</td>
<td>(0,v,0)</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>Coordinates</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>Positions</td>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2)’ +</td>
<td>(0,0,0)</td>
<td>(0,v,0)</td>
<td>(0,v,0)</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
<td>(0,0,0)</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] \( p_{\text{4m}^2} \) \( 4\text{m}'\text{m}' \)
Along [1,0,0] \( c1\text{m}11' \)
Along [1,1,0] \( p_{2\text{a}^*} \) \( 2\text{m}'\text{m}' \)

\( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)

Origin at 0,1/2,z
Origin at x,0,0

Origin at x,x,0

Origin at x,0,0

Origin at x,0,0
Origin on $\overline{4}m'2$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0) +$ set

$(1) \ 1$

$(2) \ 2 \quad 0,0,z\quad (2_z|0,0,0)$

$(3) \ \overline{4}^+ \quad 0,0,z; 0,0,0\quad (4_z|0,0,0)'$

$(4) \ \overline{4}^+ \quad 0,0,z; 0,0,0\quad (4_z^{-1}|0,0,0)'$

$(5) \ m' \ x,0,z\quad (m_y|0,0,0)'$

$(6) \ m' \ 0,y,z\quad (m_x|0,0,0)'$

$(7) \ 2 \quad x,x,0\quad (2_{xy}|0,0,0)$

$(8) \ 2 \quad x,x,0\quad (2_{xy}|0,0,0)$

For $(1/2,1/2,1/2) +$ set

$(1) \ t' \ (1/2,1/2,1/2)$

$(2) \ 2' \quad (0,0,1/2) \quad 1/4,1/4,z\quad (2_z|1/2,1/2,1/2)'$

$(3) \ \overline{4}^+ \quad 1/2,0,z; 1/2,0,1/4\quad (4_z|1/2,1/2,1/2)$

$(4) \ \overline{4}^+ \quad 0,1/2,z; 0,1/2,1/4\quad (4_z^{-1}|1/2,1/2,1/2)$

$(5) \ n \ (1/2,0,1/2) \quad x,1/4,z\quad (m_y|1/2,1/2,1/2)$

$(6) \ n \ (0,1/2,1/2) \quad 1/4,y,z\quad (m_x|1/2,1/2,1/2)$

$(7) \ 2' \quad (1/2,1/2,0) \quad x,x,1/4\quad (2_{xy}|1/2,1/2,1/2)'$

$(8) \ 2' \quad x,x+1/2,1/4\quad (2_{xy}|1/2,1/2,1/2)'$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(1/2,1/2,1/2)’ +</th>
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<tbody>
<tr>
<td>16 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 i .m’. x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
<td>0,x,z [0,u,w]</td>
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<tr>
<td>8 h .2’ x,x+1/2,1/4 [u,u,w]</td>
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<td>x+1/2,x,3/4 [u,u,w]</td>
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<tr>
<td>8 g .2 x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
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<tr>
<td>4 f 2m’m’. 0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>4 e 2m’m’. 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>2 d 4m’2’ 0,1/2,3/4 [0,0,w]</td>
<td>0,1/2,1/4 [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>2 c 4m’2’ 0,0,1/2 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b 4m’2’ 0,0,0 [0,0,0]</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>2 a 4m’2’ 0,0,0 [0,0,0]</td>
<td></td>
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</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_{4}’4m’m’

a’ = (a - b)/2  b’ = (a + b)/2

Origin at 0,0,z

Along [1,0,0] c_{p}.1m’1

a* = b  b* = c

Origin at x,0,0

Along [1,1,0] p_{2a}.2m’m’

a* = -c/2  b* = (-a + b)/2

Origin at x,x,0

Along [1,0,0] p_{2a}.2m’m’

a’ = (a - b)/2  b’ = (a + b)/2

Origin at 0,0,z
Origin on $\overline{4}c2_1$

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
   
2. $2$ ($0,0,z$)
   
3. $\overline{4}$ ($0,0,0$)
   
4. $\overline{4}$ ($0,0,z$)

5. $c$ ($0,0,1/2$) ($0,0,1/2$)
   
6. $c$ ($0,0,1/2$) ($0,0,1/2$)

7. $2$ ($0,0,0$)

8. $2$ ($0,0,0$)

For $(1/2,1/2,1/2)$ + set

1. $t$ ($1/2,1/2,1/2$)

2. $2$ ($0,0,1/2$) ($1/2,1/2,1/2$)

3. $\overline{4}$ ($0,0,1/2$) ($1/2,1/2,1/2$)

4. $\overline{4}$ ($0,0,1/2$) ($1/2,1/2,1/2$)

5. $a$ ($1/2,0,0$) ($1/2,1/2,1/2$)

6. $b$ ($0,1/2,0$) ($1/2,1/2,1/2$)

7. $2$ ($1/2,1/2,0$) ($1/2,1/2,0$)

8. $2$ ($1/2,1/2,0$) ($1/2,1/2,0$)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<td>[u,v,w]</td>
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<td>[v,u,w]</td>
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<td>(4) y,x,z</td>
<td>[v,u,w]</td>
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<td>[u,v,w]</td>
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<td>(6) x,y,z+1/2</td>
<td>[v,u,w]</td>
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<td>(7) y,x,z</td>
<td>[v,u,w]</td>
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<tr>
<td>(8) y,x,z</td>
<td>[v,u,w]</td>
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<table>
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<tr>
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<tr>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
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<tr>
<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<tr>
<td>(5) x,y,z+1/2 [u,v,w]</td>
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<td>(6) x,y,z+1/2 [v,u,w]</td>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
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<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'm'm
a^* = (a - b)/2   b^* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2m1m'
a^* = b/2   b^* = c/2
Origin at x,0,0

Along [1,1,0] p2m1m'
a^* = (-a + b)/2   b^* = c/2
Origin at x,x,0
I4c21'  
120.2.979

Tetragonal

1'

Origin on $\overline{4}c_{2,1}'$

Asymmetric unit

$0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/4$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1  
(1|0,0,0)

(2) 2 0,0,z  
(2z|0,0,0)

(3) $\overline{4}^+$ 0,0,z; 0,0,0  
($4_z|0,0,0$)

(4) $\overline{4}^-$ 0,0,z; 0,0,0  
($4_z^{-1}|0,0,0$)

(5) c (0,0,1/2) x,0,z  
($m_y|0,0,1/2$)

(6) c (0,0,1/2) 0,y,z  
($m_x|0,0,1/2$)

(7) 2 x,x,1/4  
($2_{xy}|0,0,1/2$)

(8) 2 x,x,1/4  
($2_{xy}|0,0,1/2$)

For $(1/2,1/2,1/2) +$ set

(1) t (1/2,1/2,1/2)  
(1|1/2,1/2,1/2)

(2) 2 (0,0,1/2) 1/4,1/4,z  
($2_z|1/2,1/2,1/2$)

(3) $\overline{4}^+$ 1/2,0,z; 1/2,0,1/4  
($4_z|1/2,1/2,1/2$)

(4) $\overline{4}^-$ 1/2,0,z; 1/2,0,1/4  
($4_z^{-1}|1/2,1/2,1/2$)

(5) a (1/2,0,0) x,1/4,z  
($m_y|1/2,1/2,0$)

(6) b (0,1/2,0) 1/4,y,z  
($m_x|1/2,1/2,0$)

(7) 2 (1/2,1/2,0) x,0  
($2_{xy}|1/2,1/2,0$)

(8) 2 x,x+1/2,0  
($2_{xy}|1/2,1/2,0$)
Continued

For \((0,0,0)\)' + set

\[(1)\] \(1'\) \(0,0,0\)
\[(1)\] \(1'\) \(0,0,0\)
\[(2)\] \(2'\) \(0,0,0\)
\[(2)\] \(2'\) \(0,0,0\)
\[(3)\] \(3'\) \(0,0,0\)
\[(3)\] \(3'\) \(0,0,0\)
\[(4)\] \(4'\) \(0,0,0\)
\[(4)\] \(4'\) \(0,0,0\)

\((\text{Generators selected})\)

\((1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.\)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 i 11'</td>
<td>(x,y,z [0,0,0])</td>
</tr>
<tr>
<td>8 h .21'</td>
<td>(x+1/2,0 [0,0,0])</td>
</tr>
<tr>
<td>8 g 2..1'</td>
<td>(0,1/2,z [0,0,0])</td>
</tr>
<tr>
<td>8 f 2..1'</td>
<td>(0,0,z [0,0,0])</td>
</tr>
<tr>
<td>8 e .21'</td>
<td>(x,1/4 [0,0,0])</td>
</tr>
<tr>
<td>4 d 2.221'</td>
<td>(0,1/2,0 [0,0,0])</td>
</tr>
<tr>
<td>4 c .4..1'</td>
<td>(0,1/2,1/4 [0,0,0])</td>
</tr>
<tr>
<td>4 b .4..1'</td>
<td>(0,1/2,0 [0,0,0])</td>
</tr>
<tr>
<td>4 a 2.221'</td>
<td>(0,0,1/4 [0,0,0])</td>
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</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Origin at (0,0,z)</th>
<th>(a^* = (a - b)/2)</th>
<th>(b^* = (a + b)/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at (x,0,0)</td>
<td>(a^* = b/2)</td>
<td>(b^* = c/2)</td>
</tr>
</tbody>
</table>

**Note:** \(\alpha = c/2\) and \(\beta = b/2\) do not apply here. Origin at \(x,x,0\).
Origin on $\overline{4}c'2$.

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0)$ + set

1. $1 (1) (0,0,0)$
2. $2 \cdot 0,0,z (2z (0,0,0))$
3. $\overline{4}c' \cdot 0,0,z; 0,0,0 (4z (0,0,0)')$
4. $\overline{4}c' \cdot 0,0,z; 0,0,0 (4z^{-1} (0,0,0)')$

5. $c' (0,0,1/2) \cdot x,0,z (m_x (0,0,1/2)')$
6. $c' (0,0,1/2) \cdot y,z (m_y (0,0,1/2)')$
7. $2 \cdot x,x,1/4 (2_{xy} (0,0,1/2))$
8. $2 \cdot x,x,1/4 (2_{xy} (0,0,1/2))$

For $(1/2,1/2,1/2)$ + set

1. $t (1/2,1/2,1/2) (1) (1/2,1/2,1/2)$
2. $2 \cdot (0,0,1/2) \cdot 1/4,1/4,z (2z (1/2,1/2,1/2))$
3. $\overline{4}c' \cdot 1/2,0,z; 1/2,0,1/4 (4z (1/2,1/2,1/2)')$
4. $\overline{4}c' \cdot 0,1/2,z; 0,1/2,1/4 (4z^{-1} (1/2,1/2,1/2)')$

5. $a' (1/2,0,0) \cdot x,1/4,z (m_y (1/2,1/2,0)')$
6. $b' (0,1/2,0) \cdot 1/4,y,z (m_x (1/2,1/2,0)')$
7. $2 \cdot (1/2,1/2,0) \cdot x,x,0 (2_{xy} (1/2,1/2,0))$
8. $2 \cdot x,x,0+1/2,0 (2_{xy} (1/2,1/2,0))$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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### Symmetry of Special Projections

Along [0,0,1] p4m'\(m'\) \(a^* = (a - b)/2\) b\(b^* = (a + b)/2\)
Along [1,0,0] p1m'1 \(a^* = b/2\) b\(b^* = c/2\)
Along [1,1,0] p2m'y' \(a^* = -(a + b)/2\) b\(b^* = c/2\)

Origin at 0,0,z Origin at x,0,0 Origin at x,x,0

---

120.3.980 - 2 - 1958
Origin on $4\text{c}2'$

Asymmetric unit \[0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/4\]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\) \hfill 2. \(2\ 0,0,z\) \hfill 3. \(4^{-}\ 0,0,z; 0,0,0\) \hfill 4. \(4^{-}\ 0,0,z; 0,0,0\)
   \((2z\ 0,0,0)\)

5. \(c\ (0,0,1/2)\ x,0,z\) \hfill 6. \(c\ (0,0,1/2)\ 0,y,z\) \hfill 7. \(2'\ x,x,1/4\) \hfill 8. \(2'\ x,x,1/4\)
   \((mz,0,0,1/2)\)

For \((1/2,1/2,1/2) + \) set

1. \(t\ (1/2,1/2,1/2)\) \hfill 2. \(2\ (0,0,1/2)\ 1/4,1/4,z\) \hfill 3. \(4^{-}\ 1/2,0,z; 1/2,0,1/4\) \hfill 4. \(4^{-}\ 0,1/2,z; 0,1/2,1/4\)
   \((2z\ 1/2,1/2,1/2)\)

5. \(a\ (1/2,0,0)\ x,1/4,z\) \hfill 6. \(b\ (0,1/2,0)\ 1/4,y,z\) \hfill 7. \(2'\ (1/2,1/2,0)\ x,x,0\) \hfill 8. \(2'\ x,x+1/2,0\)
   \((mz,1/2,1/2,0)\)

\(120.4.981 - 1 - 1959\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>(3) y,x,z [v,u,w]</td>
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<td>(5) x,y,z+1/2 [u,v,w]</td>
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<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td>(8) x,y,z+1/2 [v,u,w]</td>
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Symmetry of Special Projections

<table>
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<tr>
<th>Origin</th>
<th>4 d 2.2' 0,1/2,0 [0,0,w]</th>
<th>1/2,0,0 [0,0,w]</th>
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<td>0,1/2,3/4 [0,0,0]</td>
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<td>4 b</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>4 a</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
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</table>

Along [0,0,1] p4mm
a⁺ = (a - b)/2 b⁺ = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2b*m1
a⁺ = b/2 b⁺ = c/2
Origin at x,0,0

Along [1,1,0] p2m*m'1
a⁺ = (-a + b)/2 b⁺ = c/2
Origin at x,x,0

Symmetry of Special Projections
Along [0,0,1] p4mm
a⁺ = (a - b)/2 b⁺ = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2b*m1
a⁺ = b/2 b⁺ = c/2
Origin at x,0,0

Along [1,1,0] p2m*m'1
a⁺ = (-a + b)/2 b⁺ = c/2
Origin at x,x,0
I4 \text{c}2' \quad 120.5.982 \quad I4 \text{c}2'

Tetragonal

Origin on $\bar{4}c2'$

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/4$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1
(2) $\bar{1}$ 0,0,z
(3) $\bar{4}$ 0,0,z; 0,0,0
(4) $\bar{4}$ 0,0,z; 0,0,0

(5) $c'$ (0,0,1/2) x,0,z
(6) $c'$ (0,0,1/2) 0,y,z
(7) $2'$ x,x,1/4
(8) $2'$ x,x,1/4

For $(1/2,1/2,1/2) +$ set

(1) t (1/2,1/2,1/2)
(2) $\bar{2}$ (0,0,1/2) 1/4,1/4,z
(3) $\bar{4}$ 1/2,0,z; 1/2,0,1/4
(4) $\bar{4}$ 0,1/2,z; 0,1/2,1/4

(5) $a'$ (1/2,0,0) x,1/4,z
(6) $b'$ (0,1/2,0) 1/4,y,z
(7) $2'$ (1/2,1/2,0) x,x,0
(8) $2'$ x,x+1/2,0

120.5.982 - 1 - 1961
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Site Symmetry</th>
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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
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<td>..2’</td>
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<td>x+1/2,x,0 [u,u,w]</td>
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<tr>
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<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
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<tr>
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<td>0,1/2,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
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<tr>
<td>8</td>
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<tr>
<td>8</td>
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<td>..2’</td>
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<td>x,x,3/4 [u,u,w]</td>
<td>x,x,3/4 [u,u,w]</td>
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<td>4.</td>
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<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4’mm’

a’ = (a - b)/2   b’ = (a + b)/2

Origin at 0,0,z

Along [1,0,0] p1m’1

a’ = b/2   b’ = c/2

Origin at x,0,0

Along [1,1,0] p2’mm’

a’ = -c/2   b’ = (-a + b)/2

Origin at x,x,0
I$_{4}$$\overline{4}$c2

120.6.983

Tetragonal

\(\overline{4}m21'\)

I$_{4}$$\overline{4}$c2

Origin on $\overline{4}c2$.

Asymmetric unit

\[0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{4}\]

Symmetry Operations

For (0,0,0) + set

(1) $1$

(2) $2 \ 0,0,z$

(3) $\overline{4} \ + \ 0,0,z; \ 0,0,0$

(4) $\overline{4} \ - \ 0,0,z; \ 0,0,0$

(5) \(c \ (0,0,1/2) \ x,0,z$

(6) \(c \ (0,0,1/2) \ y,0,z$

(7) $\overline{4} \ + \ x,x,1/4$

(8) $\overline{4} \ - \ x,x,1/4$

For (1/2,1/2,1/2) + set

(1) $t' \ (1/2,1/2,1/2)$

(2) $2' \ (0,0,1/2) \ 1/4,1/4,z$

(3) $\overline{4} \ + \ 1/2,0,z; \ 1/2,0,1/4$

(4) $\overline{4} \ - \ 0,1/2,z; \ 0,1/2,1/4$

(5) \(a' \ (1/2,0,0) \ x,1/4,z$

(6) \(b' \ (0,1/2,0) \ 1/4,y,z$

(7) $\overline{4} \ + \ 1/2,1/2,0$ \(x,x,0$

(8) $\overline{4} \ - \ x,x+1/2,0$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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</table>

Symmetry of Special Projections

Along [0,0,1] p₄’-4mm
a’ = (a - b)/2  b’ = (a + b)/2
Origin at 0,1/2,z

Along [1,0,0] p₂₂₁m’1
a’ = b/2  b’ = c/2
Origin at x,0,0

Along [1,1,0] p₂₂’2m’m’
a’ = -c/2  b’ = (-a + b)/2
Origin at x,x,0
Origin on $\overline{4}c'2'_t$.

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/4$

**Symmetry Operations**

For $(0,0,0) + \text{set}$

1. $1$
2. $2 \ 0,0,z$
3. $\overline{4} \ 0,0,0; 0,0,0$
4. $\overline{4} \ 0,0,0; 0,0,0$

$(5) \ c'(0,0,1/2) \ x,0,z$

$(6) \ c'(0,0,1/2) \ 0,y,z$

$(7) \ 2' \ x,x,1/4$

$(8) \ 2' \ x,x,1/4$

For $(1/2,1/2,1/2)' + \text{set}$

1. $t'(1/2,1/2,1/2)$
2. $2' (0,0,1/2) \ 1/4,1/4,0$
3. $\overline{4}' \ 1/2,0,z; 1/2,0,1/4$
4. $\overline{4}' \ 0,1/2,z; 0,1/2,1/4$

$(5) \ a (1/2,0,0) \ x,1/4,z$

$(6) \ b (0,1/2,0) \ 1/4,y,z$

$(7) \ 2 (1/2,1/2,0) \ x,0$

$(8) \ 2 \ x,x+1/2,0$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<tr>
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<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z+1/2 [v,u,w]</td>
</tr>
<tr>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8 h 2</td>
<td>x,x+1/2,0 [u,u,0]</td>
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<td>x,x+1/2,0 [u,u,0]</td>
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<td>x+1/2,x,0 [u,u,0]</td>
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<tr>
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<td>x+1/2,x,0 [u,u,0]</td>
</tr>
<tr>
<td>8 g 2</td>
<td>0,1/2,z [0,0,w]</td>
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<td>1/2,0,z [0,0,w]</td>
</tr>
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</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 f 2</td>
<td>0,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
</tr>
<tr>
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<td>0,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 e ..2'</td>
<td>x,x,1/4 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/4 [u,u,w]</td>
</tr>
<tr>
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<td>x,x,1/4 [u,u,w]</td>
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<tr>
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<td>x,x,3/4 [u,u,w]</td>
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<tr>
<td>4 d 2.22</td>
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<td>1/2,0,0 [0,0,0]</td>
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<tr>
<td>4 c ..4'</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
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<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b ..4'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 2.2'2'</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p'(4m'4m')
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,1/2,z

Along [1,0,0] p1m'1
\[ a^* = b/2 \quad b^* = c/2 \]
Origin at x,0,0

Along [1,1,0] p2a, 2m'm'
\[ a^* = -c/2 \quad b^* = (-a + b)/2 \]
Origin at x,x,0

\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,1/2,z
I4\( \text{2m} \)

```
121.1.985
```

### Origin
on \( \text{42m} \)

### Asymmetric unit

\[
0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2; \quad x < y
\]

### Symmetry Operations

For \((0,0,0)\) + set

1. \(1\)
   
   \[ (1) 0,0,0 \]

2. \(2\)
   
   \[ (2) 0,0,z \]

3. \(\bar{4}\)
   
   \[ (3) \bar{4}, 0,0,z; 0,0,0 \]

4. \(4\)
   
   \[ (4) 4, 0,0,z; 0,0,0 \]

For \((1/2,1/2,1/2)\) + set

1. \(1\)
   
   \[ (1) 0,0,0 \]

2. \(2\)
   
   \[ (2) 0,0,1/2 \]

3. \(\bar{4}\)
   
   \[ (3) \bar{4}, 1/2,0,z; 1/2,0,1/4 \]

4. \(4\)
   
   \[ (4) 4, 1/2,0,z; 0,1/2,1/4 \]

For \((1/2,1/2,1/2)\) + set

1. \(1\)
   
   \[ (1) 0,0,0 \]

2. \(2\)
   
   \[ (2) 0,0,1/2 \]

3. \(\bar{4}\)
   
   \[ (3) \bar{4}, 1/2,0,z; 1/2,0,1/4 \]

4. \(4\)
   
   \[ (4) 4, 1/2,0,z; 0,1/2,1/4 \]

5. \(2\)
   
   \[ (5) 1/2,0,0 \]

6. \(2\)
   
   \[ (6) 1/2,0,0 \]

7. \(c\)
   
   \[ (7) c, 0,1/2 \]

8. \(n\)
   
   \[ (8) n, 1/2,1/2,1/2 \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>j</td>
<td>16</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>i</td>
<td>8</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>h</td>
<td>8</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>g</td>
<td>8</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>f</td>
<td>8</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>e</td>
<td>4</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>d</td>
<td>4</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>c</td>
<td>4</td>
<td>x,2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>b</td>
<td>2</td>
<td>x,2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>a</td>
<td>2</td>
<td>x,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'm'm

\[
a^* = (a - b)/2 \quad b^* = (a + b)/2
\]

Origin at 0,0,z

Along [1,0,0] c2m'm'

\[
a^* = b \quad b^* = c
\]

Origin at x,0,0

Along [1,1,0] p1m11'

\[
a^* = (-a + b)/2 \quad b^* = c/2
\]

Origin at x,x,0
I\textsuperscript{4}2m1'  
121.2.986

\begin{align*}
\text{Origin on } & \overline{4}2m1' \\
\text{Asymmetric unit} & 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \\
\text{Symmetry Operations} & \\
\text{For } (0,0,0) + \text{ set} & \\
(1) & 1 \\
(2) & 2 \ 0,0,z \ \\
(3) & \overline{4} \ 0,0,z; 0,0,0 \\
(4) & \overline{4} \ 0,0,z; 0,0,0 \\
\text{For } (1/2,1/2,1/2) + \text{ set} & \\
(1) & t (1/2,1/2,1/2) \\
(2) & 2 \ (0,0,1/2) \ 1/4,1/4,z \\
(3) & \overline{4} \ 1/2,0,z; 1/2,0,1/4 \\
(4) & \overline{4} \ 0,1/2,z; 0,1/2,1/4 \\
\end{align*}
Continued

For (0,0,0)' + set

(1) 1'  
(2) 2' 0,0,z  
(3) 4' 0,0,z; 0,0,0  
(4) 4' 0,0,z; 0,0,0  

For (1/2,1/2,1/2)' + set

(1) 1' (1/2,1/2,1/2)  
(2) 2' (0,0,1/2) 1/4,1/4,z  
(3) 4' 1/2,0,0; 1/2,1/4,1/4  
(4) 4' 0,1/2,0; 0,1/2,1/4  

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

\[
\begin{array}{cccc}
16 & j & 11' & (1) x,y,z [0,0,0] \\
& & & (2) \bar{x},\bar{y},z [0,0,0] \\
& & & (3) y,\bar{x},\bar{z} [0,0,0] \\
& & & (4) \bar{y},x,\bar{z} [0,0,0] \\
& & & (5) \bar{x},y,z [0,0,0] \\
& & & (6) x,y,z [0,0,0] \\
& & & (7) \bar{y},x,\bar{z} [0,0,0] \\
& & & (8) y,x,\bar{z} [0,0,0]
\end{array}
\]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  
Along [1,0,0] c2mm1'  
Along [1,1,0] p1m11'  

a* = (a - b)/2  
b* = (a + b)/2

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0

2 \text{a} 42m1' 0,0,0 [0,0,0]
Origin on $\overline{4}2'm$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1
(1) 0,0,0
(5) 2' 0,y,0
(2,y,0,0)' (2) 2' 0,0,z
(2,z,0,0)
(6) 2' x,0,0
(2,x,0,0)'
(7) m x,x,z
(8) m x,x,z
(m,x,0,0) (m,x,0,0)'

For $(1/2,1/2,1/2) +$ set

(1) t (1/2,1/2,1/2)
(1) 1/2,1/2,1/2
(5) 2' (0,1/2,0) 1/4,y,1/4
(2,y,1/2,1/2; 1/2,1/2,1/2)'
(6) 2' (1/2,0,0) x,1/4,1/4
(2,x,1/2,1/2; 1/2,1/2,1/2)'
(7) c (0,0,1/2) x+1/2,x,z
(8) n (1/2,1/2,1/2) x,x,z
(m,x,1/2,1/2; 1/2,1/2,1/2)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 i m</td>
<td>x,x,z [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>8 h</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 g .2'</td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
</tr>
<tr>
<td>8 f .2'</td>
<td>x,0,0 [0,v,w]</td>
<td>x,0,0 [0,v,w]</td>
</tr>
<tr>
<td>4 e 2.mm</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 d 4'..</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 c 22'2'</td>
<td>0,1/2,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td>2 b 4'2'm</td>
<td>0,0,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>2 a 4'2'm</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
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</tbody>
</table>

#### Coordinates

<table>
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<tr>
<th>16 j 1</th>
<th>(0,0,0) +</th>
<th>(1/2,1/2,1/2) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(8) y,x,z [v,u,w]</td>
<td>(9) y,x,z [v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p4m'm'
  - \(a^* = (a - b)/2\)
  - \(b^* = (a + b)/2\)
  - Origin at 0,0,z

- Along [1,0,0] c2m'm'
  - \(a^* = b\)
  - \(b^* = c\)
  - Origin at x,0,0

- Along [1,1,0] p1m11'
  - \(a^* = -(a + b)/2\)
  - \(b^* = c/2\)
  - Origin at x,x,0
Origin on $\bar{4}2m'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

Symmetry Operations

For $(0,0,0) + \text{set}$

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1 \quad (1) \quad 0,0,0$</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td>2</td>
<td>$2 \quad (1) \quad 0,0,z \quad (2z,0,0,0)$</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>3</td>
<td>$4' \quad 0,0,z; 0,0,0 \quad (4z,0,0,0)'$</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>4</td>
<td>$\bar{4}2m' \quad 0,0,z; 0,0,0 \quad (4z,1,0,0)'$</td>
<td>$0,0,z$</td>
</tr>
</tbody>
</table>

For $(1/2,1/2,1/2) + \text{set}$

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$t \quad (1) \quad 1/2,1/2,1/2 \quad (1/2,1/2,1/2)$</td>
<td>$1/2,1/2,1/2$</td>
</tr>
<tr>
<td>2</td>
<td>$2 \quad (0,0,1/2) \quad 1/4,1/4,z \quad (2z,1/2,1/2,1/2)$</td>
<td>$1/4,1/4,z$</td>
</tr>
<tr>
<td>3</td>
<td>$4' \quad 1/2,0,z; 1/2,0,1/4 \quad (4z,1/2,1/2,1/2)'$</td>
<td>$1/2,0,z$</td>
</tr>
<tr>
<td>4</td>
<td>$\bar{4}2m' \quad 0,1/2,z; 0,1/2,1/4 \quad (4z,1/2,1/2,1/2)'$</td>
<td>$0,1/2,z$</td>
</tr>
</tbody>
</table>

121.4.988 - 1 - 1973
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 j</td>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>16 j</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 j</td>
<td>(3) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>16 j</td>
<td>(4) y,x,z [v,u,w]</td>
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</tr>
<tr>
<td>16 j</td>
<td>(5) x,y,z [u,v,w]</td>
<td></td>
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<tr>
<td>8 i</td>
<td>(6) x,y,z [u,v,w]</td>
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</tr>
<tr>
<td>8 i</td>
<td>(7) y,x,z [v,u,w]</td>
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<td>8 i</td>
<td>(8) y,x,z [v,u,w]</td>
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</tr>
<tr>
<td>8 h</td>
<td>x,x,z [u,u,w]</td>
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</tr>
<tr>
<td>8 h</td>
<td>x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>8 h</td>
<td>x,x,z [u,u,w]</td>
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<tr>
<td>8 f</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td>8 f</td>
<td>x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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<tr>
<td>8 f</td>
<td>x,y,z [u,v,w]</td>
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<tr>
<td>8 f</td>
<td>x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>4 e</td>
<td>0,0,z [0,0,w]</td>
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<tr>
<td>4 d</td>
<td>0,1/2,1/4 [0,0,0]</td>
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</tr>
<tr>
<td>4 c</td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p4mm
- Along [1,0,0] c2m'm'
- Along [1,1,0] p1m'1

**a** = (a - b)/2   **b** = (a + b)/2
Origin at 0,0,z

**a** = b   **b** = c
Origin at x,0,0

**a** = (-a + b)/2   **b** = c/2
Origin at x,x,0
Origin on $\overline{4}2'm'$

Asymmetric unit $\begin{cases} 0 \leq x \leq 1/2; \\ 0 \leq y \leq 1/2; \\ 0 \leq z \leq 1/2; \\ x \leq y \end{cases}$

Symmetry Operations

For $(0,0,0) +$ set

1. $\begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix}$
2. $\begin{pmatrix} 2 \\ 0,0,z \\ 2_z,0,0,0 \end{pmatrix}$
3. $\begin{pmatrix} 4^- \\ 0,0,z; 0,0,0 \\ 4_z,0,0,0 \end{pmatrix}$
4. $\begin{pmatrix} 4^- \\ 0,0,z; 0,0,0 \\ 4_z^{-1},0,0,0 \end{pmatrix}$

For $(1/2,1/2,1/2) +$ set

1. $\begin{pmatrix} t \\ 1/2,1/2,1/2 \end{pmatrix}$
2. $\begin{pmatrix} 2 \\ 0,0,1/2 \\ 1/4,1/4,z \\ 2_z,1/2,1/2,1/2 \end{pmatrix}$
3. $\begin{pmatrix} 4^- \\ 1/2,0,z; 1/2,0,1/4 \\ 4_z,1/2,1/2,1/2 \end{pmatrix}$
4. $\begin{pmatrix} 4^- \\ 0,1/2,z; 0,1/2,1/4 \\ 4_z^{-1},1/2,1/2,1/2 \end{pmatrix}$

121.5.989 - 1 - 1975
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
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| 16 | j | 1 | (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] | (3) y,x,z [v,u,w] | (4) y,x,z [v,u,w] |
| 8  | i | .m' | x,x,z [u,u,w] | x,x,z [u,u,w] | x,x,z [u,u,w] | x,x,z [u,u,w] |
| 8  | h | 2.. | 0,1/2,z [0,0,w] | 1/2,0,z [0,0,w] | 0,1/2,z [0,0,w] | 1/2,0,z [0,0,w] |
| 8  | g | .2'. | x,0,1/2 [0,v,w] | x,0,1/2 [0,v,w] | 0,x,1/2 [v,0,w] | 0,x,1/2 [v,0,w] |
| 8  | f | .2'. | x,0,0 [0,v,w] | x,0,0 [0,v,w] | 0,x,0 [v,0,w] | 0,x,0 [v,0,w] |
| 4  | e | 2.m'm' | 0,0,z [0,0,w] | 0,0,z [0,0,w] |               |               |
| 4  | d | .4.. | 0,1/2,1/4 [0,0,w] | 0,1/2,3/4 [0,0,w] |               |               |
| 4  | c | 22'2'. | 0,1/2,0 [0,0,w] | 1/2,0,0 [0,0,w] |               |               |
| 2  | b | 42'm' | 0,0,1/2 [0,0,w] |               |               |               |
| 2  | a | 42'm' | 0,0,0 [0,0,w] |               |               |               |

### Symmetry of Special Projections

Along [0,0,1] p4mm'  
Along [1,0,0] c2mm'  
Along [1,1,0] p1m1

\[
a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2}
\]

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x,0
**Origin** on $\overline{4}2m$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y$

**Symmetry Operations**

For $(0,0,0)$ + set

1. $1$
   1. $(0,0,0)$

2. $0,0,z$
   2. $(2z,0,0,0)$

3. $\begin{array}{c} 4^- \quad 0,0,z; 0,0,0 \\ (4_z,0,0,0) \end{array}$

4. $\begin{array}{c} 4^- \quad 0,0,z; 0,0,0 \\ (4_z^{-1},0,0,0) \end{array}$

For $(1/2,1/2,1/2)'$ + set

1. $t' (1/2,1/2,1/2)$
   1. $(1/2,1/2,1/2)$

2. $(0,0,1/2)$
   2. $(1/2,1/2,1/2)'$

3. $\begin{array}{c} 4^-' \quad 1/2,0,z; 1/2,0,1/4 \\ (4_z,1/2,1/2,1/2)' \end{array}$

4. $\begin{array}{c} 4^-' \quad 0,1/2,z; 0,1/2,1/4 \\ (4_z^{-1},1/2,1/2,1/2)' \end{array}$

(1) $0,0,0$

(2) $x,0,0$

(3) $x,x,z$

(4) $x,y,0$

(5) $x,y,1/4$

(6) $x,1/4,1/4$

(7) $x+1/2,x,1/4$

(8) $x+1/2,1/4$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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Symmetry of Special Projections

Along [0,0,1]   p,, 4m’m’    Along [1,0,0] c2m’m’    Along [1,1,0] p1m11’

\(a^* = (a - b)/2\) \(b^* = (a + b)/2\) \(a^* = b\) \(b^* = c\) \(a^* = (-a + b)/2\) \(b^* = c/2\)

Origin at 1/2,0,z Origin at x,0,0 Origin at x,x,0
**Origin** on $\overline{4}2'm$

**Asymmetric unit**
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1\)
   
   \((1) 1\)
   \((1) 0,0,0\)

2. \(2\)
   
   \((2) 2\)
   \((2) 0,0,z\)
   \((2_x, 0, 0, 0)\)

3. \(\overline{4}^+\)
   
   \((3) \overline{4}^+\)
   \((3) 0,0,0; 0,0,0\)
   \((4, z, 0, 0, 0)\)

4. \(\overline{4}^-\)
   
   \((4) \overline{4}^-\)
   \((4) 0,0,0; 0,0,0\)
   \((4_z, 0, 0, 0)\)

For \((1/2,1/2,1/2)\) + set

1. \(t'\)
   
   \((1) t'\)
   \((1) 1/2,1/2,1/2\)
   \((1/2,1/2,1/2)\)

2. \(2'\)
   
   \((2) 2'\)
   \((2) (0,0,1/2); 1/4,1/4,z\)
   \((2_2, 1/2, 1/2, 1/2)\)

3. \(\overline{4}^+\)
   
   \((3) \overline{4}^+\)
   \((3) 1/2,0,0; 1/2,0,1/4\)
   \((4_z, 1/2, 1/2, 1/2)\)

4. \(\overline{4}^-\)
   
   \((4) \overline{4}^-\)
   \((4) 0,1/2,z; 0,1/2,1/4\)
   \((4_z, 1/2, 1/2, 1/2)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>.2'</td>
<td>x,0,1/2 [0,v,w]</td>
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<td>8 f</td>
<td>.2'</td>
<td>x,0,0 [0,v,w]</td>
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<tr>
<td>2 b</td>
<td>4'2'm</td>
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<td>4'2'm</td>
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Symmetry of Special Projections

Along [0,0,1] p,4m'4m'  
\( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  
Origin at 0,0,z

Along [1,0,0] c,2'2mm'  
\( a^* = -c \)  \( b^* = b \)  
Origin at x,0,0

Along [1,1,0] p1m11'  
\( a^* = (-a + b)/2 \)  \( b^* = c/2 \)  
Origin at x,x,0
Origin on $\overline{4}'2m'$

Asymmetric unit  
0 ≤ $x$ ≤ 1/2;  
0 ≤ $y$ ≤ 1/2;  
0 ≤ $z$ ≤ 1/2;  
x ≤ $y$

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1) 0,0,0

(2) 2 0,0,z  
(2) 0,0,0  
(2) $z$,0,0,0

(3) $\overline{4}'$ 0,0,z; 0,0,0  
(3) $\overline{4}'$ 0,0,0  
(4) $\overline{4}'$ 0,0,0; 0,0,0

For (1/2,1/2,1/2)' + set

(1) $t'$ (1/2,1/2,1/2)  
(1) 1/2,1/2,1/2

(2) 2' (0,0,1/2)  
(2) 1/4,1/4,z  
(2) $z$,1/4,1/4

(3) $\overline{4}'$ 1/2,0,z; 1/2,0,1/4  
(3) $\overline{4}'$ 1/2,1/2,1/2  
(4) $\overline{4}'$ 1/2,1/2,1/2

(5) 2' (0,1/2,0)  
(5) 1/4,y,1/4  
(5) $y$,1/4,1/4

(6) 2' (1/2,0,0)  
(6) x,1/4,1/4  
(6) $x$,1/4,1/4

(7) c (0,0,1/2)  
(7) x+1/2,$z$,1/2  
(7) $m_x$,1/2,1/2,1/2

(8) n (1/2,1/2,1/2)  
(8) $x$,x,z  
(8) $m_x$,1/2,1/2,1/2
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>(1/2,1/2,1/2)' +</td>
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Coordinates

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Symmetry of Special Projections

Along [0,0,1] \( p_{2} \cdot 4mm \) \( a^{*} = (a - b)/2 \) \( b^{*} = (a + b)/2 \)
Origin at 0,0,z

Along [1,0,0] \( c_{2} \cdot 2m'm' \) \( a^{*} = b \) \( b^{*} = c \)
Origin at 0,0,0

Along [1,1,0] \( p_{2z} \cdot 1m'1 \) \( a^{*} = -(a + b)/2 \) \( b^{*} = c/2 \)
Origin at x,x,0
Origin on $\text{4}2\text{m}'$

Asymmetric unit $0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2; \quad x < y$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
   
2. $2 \cdot 0,0,z$
   
3. $\text{4}$ $0,0,z; 0,0,0$
   
4. $\text{4}$ $0,z; 0,0,0$

5. $2' 0,y,0$
   
6. $2' x,0,0$

7. $\text{m'} x,x,z$
   
8. $\text{m'} x,x,z$

For $(1/2,1/2,1/2)'$ + set

1. $t' (1/2,1/2,1/2)$
   
2. $2' (0,0,1/2) 1/4,1/4,z$
   
3. $\text{4}$ $1/2,0,z; 1/2,0,1/4$
   
4. $\text{4}$ $0,1/2,z; 0,1/2,1/4$

5. $2 (0,1/2,0) 1/4,y,1/4$
   
6. $2 (1/2,0,0) x,1/4,1/4$
   
7. $c (0,0,1/2) x+1/2,x,z$
   
8. $n (1/2,1/2,1/2) x,x,z$

121.9.993 - 1 - 1983
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

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</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
</tbody>
</table>

| 8 i .m'     | x,x,z [u,u,w] |
| 8 h 2..    | 0,1/2,z [0,0,w] |
| 8 g .2'.   | x,0,1/2 [0,v,w] |
| 8 f .2'.   | x,0,0 [0,v,w] |
| 4 e 2.m'   | 0,0,z [0,0,w] |
| 4 d 4'     | 0,1/2,1/4 [0,0,0] |
| 4 c 22'2'  | 0,1/2,0 [0,0,w] |
| 2 b 42'm'  | 0,0,1/2 [0,0,w] |
| 2 a 42'm'  | 0,0,0 [0,0,w] |

Symmetry of Special Projections

- Along [0,0,1] \( p_{14} \), 4m'm'
  \( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)
- Origin at 1/2,0,z

- Along [1,0,0] \( c_{14} \), 2'mm'
  \( a^* = -c \) \( b^* = b \)
- Origin at 0,0,0

- Along [1,1,0] \( p_{22} \), 1m'
  \( a^* = -(a + b)/2 \) \( b^* = c/2 \)
- Origin at x,x,0
Origin on 4

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/8

Symmetry Operations

For (0,0,0) + set

1.
   (1) 1
      (1|0,0,0)

2.
   (2) 2 0,0,z
       (2|0,0,0)

3.
   (3) 4' 0,0,z; 0,0,0
       (4|0,0,0)

4.
   (4) 4' 0,0,z; 0,0,0
       (4|0,0,0)

For (1/2,1/2,1/2) + set

1.
   (1) t (1/2,1/2,1/2)
      (1|1/2,1/2,1/2)

2.
   (2) 2 (0,0,1/2) 1/4,1/4,z
       (2|1/2,1/2,1/2)

3.
   (3) 4' 1/2,0,z; 1/2,0,1/4
       (4|1/2,1/2,1/2)

4.
   (4) 4' 0,1/2,z; 0,1/2,1/4
       (4|1/2,1/2,1/2)

5.
   (5) 2 1/4,y,3/8
       (2|1/2,0,3/4)

6.
   (6) 2 (1/2,0,0) x,0,3/8
       (2|1/2,0,3/4)

7.
   (7) d (1/4,-1/4,3/4) x+1/4,x,z
       (m|1/2,0,3/4)

8.
   (8) d (1/4,1/4,3/4) x+1/4,x,z
       (m|1/2,0,3/4)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
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<tr>
<th>Multiplicity</th>
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<td>(1/2,1/2,1/2) +</td>
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<td>(1) x,y,z [u,v,w]</td>
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<td>(2) x̅,y,z [u̅,v̅,w]</td>
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(1) x,y,z [u,v,w]  
(2) x̅,y,z [u̅,v̅,w]  
(3) y,x,z [v,u,w]  
(4) y,z [v,0,w]  
(5) x,y,z [v,u,w]  
(6) x,y,z [v,u̅,w]  
(7) y,x,z [v,u,w]  
(8) y,x,z [v,u̅,w]  

8 d .2. x,1/4,1/8 [u,0,0]  
8 c 2.. 0,0,z [0,0,w]  
4 b 4.. 0,0,1/2 [0,0,w]  
4 a 4.. 0,0,0 [0,0,w]  

Symmetry of Special Projections

Along [0,0,1] p4'g'm  
a* = (a - b)/2  
b* = (a + b)/2  
Origin at 0,0,z

Along [1,0,0] c2m'm'  
a* = b  
b* = c  
Origin at x,0,3/8

Along [1,1,0] c1m'1  
a* = (-a + b)/2  
b* = c/2  
Origin at x,x,0
Origin on $\bar{4} 1'$

Asymmetric unit

$0 \leq x \leq 1/2$; $0 \leq y \leq 1$; $0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
   
   $1' (0,0,0)$

2. $2$
   
   $0,0,z$
   
   $(2_z,0,0,0)$

3. $\bar{4}$
   
   $0,0,z$; $0,0,0$
   
   $(4_z,0,0,0)$

For $(1/2,1/2,1/2)$ + set

1. $t$
   
   $(1/2,1/2,1/2)$

2. $2$
   
   $(0,0,1/2)$; $1/4,1/4,z$
   
   $(2_z,1/2,1/2,1/2)$

3. $\bar{4}$
   
   $1/2,0,z$; $1/2,0,1/4$
   
   $(4_z,1/2,1/2,1/2)$

4. $\bar{4}$
   
   $0,1/2,z$; $0,1/2,1/4$
   
   $(4_z^{-1},0,0,0)$
For (0,0,0)' + set

(1) 1' (2) 2' 0,0,z (3) 4' 0,0,z; 0,0,0 (4) 4' 0,0,z; 0,0,0
(1,0,0,0)' (4z,0,0,0)' (4z,0,0,0)' (4z,0,0,0)'

(5) 2' (0,1/2,0) 0,y,1/8 (2z,0,1/2,1/4)'

(6) 2' x,1/4,1/8 (7) d' (1/4,1/4,1/4) x+1/4,x,z (8) d' (1/4,1/4,1/4) x-1/4,x,z
(2z,0,1/2,1/4) (m_y) 0,1/2,1/4) (m_y) 0,1/2,1/4)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (2) 2' (0,0,1/2) 1/4,1/4,z (3) 4' 1/2,0,z; 1/2,0,1/4 (4) 4' 0,1/2,z; 0,1/2,1/4
(1,1/2,1/2,1/2) (2z,1/2,1/2,1/2) (4z,1/2,1/2,1/2) (4z,1/2,1/2,1/2)'

(5) 2' 1/4,y,3/8 (2z,1/2,0,3/4)'

(6) 2' (1/2,0,0) x,0,3/8 (7) d' (1/4,-1/4,3/4) x+1/4,x,z (8) d' (1/4,1/4,3/4) x+1/4,x,z
(2z,1/2,0,3/4) (m_x) 1/2,0,3/4) (m_x) 1/2,0,3/4)'

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5): 1'.

Positions

Multiplicity
Wyckoff letter
Site Symmetry

(0,0,0) + (1/2,1/2,1/2) + 
(0,0,0)' + (1/2,1/2,1/2)' +

16 e 11' (1) x,y,z [0,0,0] (2) x,y,z [0,0,0]
(3) y,x,z [0,0,0] (4) y,x,z [0,0,0]
(5) x,y+1/2,z+1/4 [0,0,0] (6) x,y+1/2,z+1/4 [0,0,0]
(7) y,x+1/2,z+1/4 [0,0,0] (8) y,x+1/2,z+1/4 [0,0,0]

8 d .2.1' x,1/4,1/8 [0,0,0] x,3/4,1/8 [0,0,0] 1/4,x,7/8 [0,0,0] 3/4,x,7/8 [0,0,0]
8 c 2..1' 0,0,z [0,0,0] 0,0,z [0,0,0] 0,1/2,z+1/4 [0,0,0] 0,1/2,z+1/4 [0,0,0]
4 b 4..1' 0,0,1/2 [0,0,0] 0,1/2,3/4 [0,0,0] 0,1/2,3/4 [0,0,0]
4 a 4..1' 0,0,0 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4gm1' Along [1,0,0] c2mm1' Along [1,1,0] c1m11'
a* = (a - b)/2 b* = (a + b)/2 a* = b b* = c a* = (-a + b)/2 b* = c/2
Origin at 0,0,z Origin at x,0,3/8 Origin at x,x,0
**Symmetry Operations**

**For (0,0,0) + set**

1. \(1 \quad (1) 0,0,0 \)
   \(1^* \quad (2) 0,0,z \)
   \(2^d \quad (3) 4^d \quad 0,0,z; 0,0,0 \)
   \(2^d \quad (4) 4^d \quad 0,0,0\)

2. \(2' \quad (5) (0,1/2,0) \quad 0,y,1/8 \)
   \(2' \quad (6) (0,1/2,1/4) \quad x,1/4,1/8 \)
   \(2' \quad (7) (1/4,-1/4,3/4) \quad x+1/4, x, z; 1/4, x, z \)
   \(2' \quad (8) (1/4,1/4,3/4) \quad x+1/4, x, z \)

**For (1/2,1/2,1/2) + set**

1. \(t \quad (1) 1/2,1/2,1/2 \)
   \(1^* \quad (2) 0,0,1/2 \quad 1/4,1/4,z \)
   \(2' \quad (3) 4^d \quad 1/2,0,z; 1/2,0,1/4 \)
   \(2' \quad (4) 4^d \quad 1/2,0,1/4\)

2. \(2' \quad (5) (1/4,y,3/8) \quad 0,3/8 \)
   \(2' \quad (6) (1/2,0,0) \quad x,0,3/8 \)
   \(2' \quad (7) (1/4,-1/4,3/4) \quad x+1/4, x, z \)
   \(2' \quad (8) (1/4,1/4,3/4) \quad x+1/4, x, z \)

**Origin on 4d**

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8 \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<tbody>
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<td>(2) x,y,z [u,v,w]</td>
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<tr>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<tr>
<td></td>
<td>(5) x+y+1/2,z+1/4 [u,v,w]</td>
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<td>(7) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4g'm'

\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]

Origin at 0,0,z

Along [1,0,0] c2m'm'

\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]

Origin at x,0,3/8

Along [1,1,0] \( \mathbf{c}_s \mathbf{1m}'1 \)

\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]

Origin at x,x,0
Origin on $\overline{4}v$

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1
    (1) $|0,0,0|

(2) 2 $0,0,z$
    (2) $2|0,0,0$

(3) $\overline{4}v$ $0,0; 0,0,0$
    $\left(\frac{4}{x},0,0,0\right)$

(4) $\overline{4}v$ $0,0; 0,0,0$
    $\left(\frac{4}{x}\right)|0,0,0\right)$

For $(1/2,1/2,1/2)$ + set

(1) t $(1/2,1/2,1/2)$
    $(1) |1/2,1/2,1/2|

(2) 2 $(0,0,1/2)$ $1/4,1/4,1/4$
    (2) $2|1/2,1/2,1/2|

(3) $\overline{4}v$ $1/2,0; 1/2,0,1/4$
    $\left(\frac{4}{x},1/2,1/2,1/2\right)$

(4) $\overline{4}v$ $0,1/2,z; 0,1/2,1/4$
    $\left(\frac{4}{x}|1/2,1/2,1/4\right)$

(5) 2 $1/4,y,3/8$
    $(2) |1/2,0,3/4|

(6) 2 $(1/2,0,0)$ $0,3/8$
    (2) $2|1/2,0,3/4|

(7) $\overline{4}v$ $1/4,-1/4,3/4$
    $\left(\frac{4}{x},1/2,0,3/4\right)$

(8) $\overline{4}v$ $1/4,1/4,3/4$
    $\left(\frac{4}{x}|1/2,0,3/4\right)$

122.4.997 - 1 - 1991
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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<td>x,y,z [u,v,w]</td>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(5) x,y+1/2,z+1/4 [u,v,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p4gm

a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] c2m'm'

a* = b  b* = c
Origin at x,0,3/8

Along [1,1,0] c1m'1

a* = (-a + b)/2  b* = c/2
Origin at x,x,0
Origin on $\overline{4}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
   $(1) \ 0,0,0$
   $(2) \ 2 \ 0,0,z$
   $(3) \ \overline{4}^+ \ 0,0,z \ 0,0,0$
   $(4) \ \overline{4}^- \ 0,0,z \ 0,0,0$
   $(5) \ 2' \ (0,1/2,0) \ 0,y,1/8$
   $(2y) \ 0,1/2,1/4)$
   $(6) \ 2' \ x,1/4,1/8$
   $(2x) \ 0,1/2,1/4)$
   $(7) \ d' \ (-1/4,1/4,1/4) \ x+1/4,x,z$
   $(m_{xy}) \ 0,1/2,1/4)$
   $(8) \ d' \ (1/4,1/4,1/4) \ x-1/4,x,z$
   $(m_{xy}) \ 0,1/2,1/4)$

For $(1/2,1/2,1/2) +$ set

1. $t \ (1/2,1/2,1/2)$
   $(1) \ 0,0,1/2$
   $(2) \ 2 \ (0,0,1/2) \ 1/4,1/4,z$
   $(3) \ \overline{4}^+ \ 1/2,0,z \ 1/2,0,1/4$
   $(4) \ \overline{4}^- \ 1/2,0,z \ 0,1/2,1/4$
   $(5) \ 2' \ 1/4,y,3/8$
   $(2y) \ 1/2,0,3/4)$
   $(6) \ 2' \ (1/2,0,0) \ x,0,3/8$
   $(2x) \ 1/2,0,3/4)$
   $(7) \ d' \ (1/4,-1/4,3/4) \ x+1/4,x,z$
   $(m_{xy}) \ 1/2,0,3/4)$
   $(8) \ d' \ (1/4,1/4,3/4) \ x+1/4,x,z$
   $(m_{xy}) \ 1/2,0,3/4)$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

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Symmetry of Special Projections

Along [0,0,1] p4'gm'  
\( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)  
Origin at 0,0,z

Along [1,0,0] c2'mm'  
\( a^* = -c \) \( b^* = b \)  
Origin at x,0,3/8

Along [1,1,0] c1m'1  
\( a^* = -(a + b)/2 \) \( b^* = c/2 \)  
Origin at x,x,0
Origin at center (4/mmm)

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≥ y

Symmetry Operations:

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(3) 4+ 0,0,z
(4z|0,0,0)

(4) 4- 0,0,z
(4z|0,0,0)

(5) 2 0,y,0
(2y|0,0,0)

(6) 2 x,0,0
(2x|0,0,0)

(7) 2 x,x,0
(2xy|0,0,0)

(8) 2 x,x,0
(2xy|0,0,0)

(9) 1 0,0,0
(1|0,0,0)

(10) m x,y,0
(mx|0,0,0)

(11) 4+ 0,0,z; 0,0,0
(4z|0,0,0)

(12) 4- 0,0,z; 0,0,0
(4z|0,0,0)

(13) m x,0,z
(mx|0,0,0)

(14) m 0,y,z
(my|0,0,0)

(15) m x,x,z
(mx|0,0,0)

(16) m x,x,z
(mx|0,0,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<tr>
<td>16 u 1</td>
<td>(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y,x,z [v,u,w]  (4) y,x,z [v,u,w]  (5) x,y,z [u,v,w]  (6) x,y,z [u,v,w]  (7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]  (9) x,y,z [u,v,w]  (10) x,y,z [u,v,w]  (11) y,x,z [v,u,w]  (12) y,x,z [v,u,w]  (13) x,y,z [u,v,w]  (14) x,y,z [u,v,w]  (15) y,x,z [v,u,w]  (16) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 t .m.</td>
<td>x,1/2,z [0,v,0]  x,1/2,z [0,v,0]  1/2,x,z [v,0,0]  1/2,x,z [v,0,0]  x,1/2,z [0,v,0]  x,1/2,z [0,v,0]  1/2,x,z [v,0,0]  1/2,x,z [v,0,0]</td>
</tr>
<tr>
<td>8 s .m.</td>
<td>x,0,z [0,v,0]  x,0,z [0,v,0]  0,x,z [v,0,0]  0,x,z [v,0,0]  x,0,z [0,v,0]  x,0,z [0,v,0]  0,x,z [v,0,0]  0,x,z [v,0,0]</td>
</tr>
<tr>
<td>8 r .m.</td>
<td>x,x,z [u,u,0]  x,x,z [u,u,0]  x,x,z [u,u,0]  x,x,z [u,u,0]  x,x,z [u,u,0]  x,x,z [u,u,0]  x,x,z [u,u,0]  x,x,z [u,u,0]</td>
</tr>
<tr>
<td>8 q .m.</td>
<td>x,y,1/2 [0,0,w]  x,y,1/2 [0,0,w]  y,x,1/2 [0,0,w]  y,x,1/2 [0,0,w]  x,y,1/2 [0,0,w]  x,y,1/2 [0,0,w]  y,x,1/2 [0,0,w]  y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 p .m.</td>
<td>x,y,0 [0,0,w]  x,y,0 [0,0,w]  y,x,0 [0,0,w]  y,x,0 [0,0,w]  x,y,0 [0,0,w]  x,y,0 [0,0,w]  y,x,0 [0,0,w]  y,x,0 [0,0,w]</td>
</tr>
<tr>
<td>4 o m2m.</td>
<td>x,1/2,1/2 [0,0,0]  x,1/2,1/2 [0,0,0]  1/2,x,1/2 [0,0,0]  1/2,x,1/2 [0,0,0]  x,1/2,1/2 [0,0,0]  x,1/2,1/2 [0,0,0]  1/2,x,1/2 [0,0,0]  1/2,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 n m2m.</td>
<td>x,1/2,0 [0,0,0]  x,1/2,0 [0,0,0]  1/2,x,0 [0,0,0]  1/2,x,0 [0,0,0]  x,1/2,0 [0,0,0]  x,1/2,0 [0,0,0]  1/2,x,0 [0,0,0]  1/2,x,0 [0,0,0]</td>
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<tr>
<td>4 m m2m.</td>
<td>x,0,1/2 [0,0,0]  x,0,1/2 [0,0,0]  0,x,1/2 [0,0,0]  0,x,1/2 [0,0,0]  x,0,1/2 [0,0,0]  x,0,1/2 [0,0,0]  0,x,1/2 [0,0,0]  0,x,1/2 [0,0,0]</td>
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<tr>
<td>4 l m2m.</td>
<td>x,0,0 [0,0,0]  x,0,0 [0,0,0]  0,x,0 [0,0,0]  0,x,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  0,x,0 [0,0,0]  0,x,0 [0,0,0]</td>
</tr>
<tr>
<td>4 k m2m.</td>
<td>x,x,1/2 [0,0,0]  x,x,1/2 [0,0,0]  x,x,1/2 [0,0,0]  x,x,1/2 [0,0,0]  x,x,1/2 [0,0,0]  x,x,1/2 [0,0,0]  x,x,1/2 [0,0,0]  x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 j m2m.</td>
<td>x,x,0 [0,0,0]  x,x,0 [0,0,0]  x,x,0 [0,0,0]  x,x,0 [0,0,0]  x,x,0 [0,0,0]  x,x,0 [0,0,0]  x,x,0 [0,0,0]  x,x,0 [0,0,0]</td>
</tr>
<tr>
<td>4 i 2mm.</td>
<td>0,1/2,z [0,0,0]  0,1/2,z [0,0,0]  0,1/2,z [0,0,0]  0,1/2,z [0,0,0]  0,1/2,z [0,0,0]  0,1/2,z [0,0,0]  0,1/2,z [0,0,0]  0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 h 4mm</td>
<td>1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 g 4mm</td>
<td>0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 f mmm.</td>
<td>0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]  0,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>
2 e mmm. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]
1 d 4/mmm 1/2,1/2,1/2 [0,0,0]
1 c 4/mmm 1/2,1/2,0 [0,0,0]
1 b 4/mmm 0,0,1/2 [0,0,0]
1 a 4/mmm 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  Along [1,0,0] p2mm1'  Along [1,1,0] p2mm1'
\(a^* = a\)  \(b^* = b\)  \(a^* = b\)  \(b^* = c\)  \(a^* = (-a + b)/2\)  \(b^* = c\)
Origin at 0,0,z  Origin at x,0,0  Origin at x,x,0
**Origin** at center (4/mmm1')

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

**Symmetry Operations**

For 1 + set

1. \( 1 \to (1|0,0,0) \)
2. \( 2 \to (2,0,0) \)
3. \( 4^+ \to (4,0,0) \)
4. \( 4^- \to (4,0,0) \)

5. \( 2 \to (2|0,0,0) \)
6. \( 2 \to (2,0,0) \)
7. \( 2 \to (2,0,0) \)
8. \( 2 \to (2,0,0) \)

9. \( \bar{1} \to (1|0,0,0) \)
10. \( m \to (m,0,0) \)
11. \( \bar{4}^+ \to (4,0,0) \)
12. \( \bar{4}^- \to (4,0,0) \)

13. \( m \to (m,0,0) \)
14. \( m \to (m,0,0) \)
15. \( m \to (m,0,0) \)
16. \( m \to (m,0,0) \)
Continued

For 1' + set

(1) 1'  
(1,0,0)

(2) 2', 0,0,0  
(1,0,0)

(3) 4', 0,0,0  
(1,0,0)

(4) 4', 0,0,0  
(1,0,0)

(5) 2', 0,0,0  
(2,0,0)

(6) 2', x,0,0  
(2,0,0)

(7) 2', x,x,0  
(2,0,0)

(8) 2', x,x,0  
(2,0,0)

(9) 1'  
(0,0,0)

(10) 2', 0,0,0  
(0,0,0)

(11) 2', 0,0,0  
(0,0,0)

(12) 2', 0,0,0  
(0,0,0)

(13) 2', 0,0,0  
(0,0,0)

(14) 2', 0,0,0  
(0,0,0)

(15) 2', 0,0,0  
(0,0,0)

(16) 2', 0,0,0  
(0,0,0)

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>u</td>
<td>1' +</td>
</tr>
<tr>
<td>16</td>
<td>u</td>
<td>1' +</td>
</tr>
<tr>
<td>8</td>
<td>t</td>
<td>1/2,x,0,0</td>
</tr>
<tr>
<td>8</td>
<td>t</td>
<td>1/2,x,0,0</td>
</tr>
<tr>
<td>8</td>
<td>s</td>
<td>0,0,0</td>
</tr>
<tr>
<td>8</td>
<td>s</td>
<td>0,0,0</td>
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<td>8</td>
<td>q</td>
<td>0,0,0</td>
</tr>
<tr>
<td>8</td>
<td>q</td>
<td>0,0,0</td>
</tr>
<tr>
<td>4</td>
<td>o</td>
<td>1/2,0,0,0</td>
</tr>
<tr>
<td>4</td>
<td>o</td>
<td>1/2,0,0,0</td>
</tr>
<tr>
<td>4</td>
<td>n</td>
<td>1/2,0,0,0</td>
</tr>
<tr>
<td>4</td>
<td>n</td>
<td>1/2,0,0,0</td>
</tr>
</tbody>
</table>
4  m  m2m.1'  x,0,1/2 [0,0,0]  \bar{x},0,1/2 [0,0,0]  0,x,1/2 [0,0,0]  0,\bar{x},1/2 [0,0,0]
4  l  m2m.1'  x,0,0 [0,0,0]  \bar{x},0,0 [0,0,0]  0,x,0 [0,0,0]  0,\bar{x},0 [0,0,0]
4  k  m.2m1'  x,x,1/2 [0,0,0]  \bar{x},x,1/2 [0,0,0]  \bar{x},x,1/2 [0,0,0]  x,\bar{x},1/2 [0,0,0]
4  j  m.2m1'  x,x,0 [0,0,0]  \bar{x},x,0 [0,0,0]  \bar{x},x,0 [0,0,0]  x,\bar{x},0 [0,0,0]
4  i  2mm.1'  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  0,1/2,\bar{z} [0,0,0]  1/2,0,\bar{z} [0,0,0]
2  h  4mm1'  1/2,1/2,z [0,0,0]  1/2,1/2,\bar{z} [0,0,0]
2  g  4mm1'  0,0,z [0,0,0]  0,0,\bar{z} [0,0,0]
2  f  mmm.1'  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]
2  e  mmm.1'  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]
1  d  4/mmm1'  1/2,1/2,1/2 [0,0,0]
1  c  4/mmm1'  1/2,1/2,0 [0,0,0]
1  b  4/mmm1'  0,0,1/2 [0,0,0]
1  a  4/mmm1'  0,0,0 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]  p4mm1'</th>
<th>Along [1,0,0]  p2mm1'</th>
<th>Along [1,1,0]  p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a   b' = b</td>
<td>a' = b   b' = c</td>
<td>a' = (-a + b)/2  b' = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

123.2.1000 - 3 - 2000
Origin at center (4/m'nm)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

Symmetry Operations

(1) 1

\[ (1\mid0,0,0) \]

(5) 2' 0,y,0

\[ (2_y\mid0,0,0)' \]

(9) 1' 0,0,0

\[ (1\mid0,0,0)' \]

(13) m x,0,z

\[ (m_x\mid0,0,0) \]

(2) 2 0,0,z

\[ (2_z\mid0,0,0) \]

(6) 2' x,0,0

\[ (2_z\mid0,0,0)' \]

(10) m' x,y,0

\[ (m_z\mid0,0,0)' \]

(14) m 0,y,z

\[ (m_y\mid0,0,0) \]

(3) 4+ 0,0,z

\[ (4_z\mid0,0,0) \]

(7) 2' x,x,0

\[ (2_{xy}\mid0,0,0)' \]

(11) 4' 0,0,z

\[ (4_z\mid0,0,0)' \]

(8) 2' x,x,0

\[ (2_{xy}\mid0,0,0)' \]

(12) 4' 0,0,z

\[ (4_z\mid0,0,0)' \]

(15) m x,x,z

\[ (m_{xy}\mid0,0,0) \]

(16) m x,x,z

\[ (m_{xy}\mid0,0,0) \]
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 u 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [v,u,w]</td>
</tr>
<tr>
<td>8 t .m.</td>
<td>x,1/2,z [0,0,0]</td>
<td>x,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>8 s .m.</td>
<td>x,0,z [0,0,0]</td>
<td>x,0,z [0,0,0]</td>
</tr>
<tr>
<td>8 r .m.</td>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>8 q m'..</td>
<td>x,y,1/2 [u,v,0]</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>8 p m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>4 o m'2m.</td>
<td>x,1/2,1/2 [0,0,0]</td>
<td>x,1/2,1/2 [0,0,0]</td>
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<tr>
<td>4 m m'2m.</td>
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<td>4 l m'2m.</td>
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<td>x,x,1/2 [u,u,0]</td>
<td>x,x,1/2 [u,u,0]</td>
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<td>4 j m'2m.</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
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<tr>
<td>4 i 2mm.</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
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<tr>
<td>2 h 4mm</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2 g 4mm</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 f m'2m.</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
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</table>
2 e mmm. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]
1 d 4/m'mm 1/2,1/2,1/2 [0,0,0]
1 c 4/m'mm 1/2,1/2,0 [0,0,0]
1 b 4/m'mm 0,0,1/2 [0,0,0]
1 a 4/m'mm 0,0,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4mm
\[
a^* = a \quad b^* = b
\]
Origin at 0,0,z

Along [1,0,0] p2mm1'
\[
a^* = b \quad b^* = c
\]
Origin at x,0,0

Along [1,1,0] p2mm1'
\[
a^* = (-a + b)/2 \quad b^* = c
\]
Origin at x,x,0
P4'/mm'm 123.4.1002

4'/mm'm

Tetragonal

Origin at center (4'/mm'm)

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad x < y \]

Symmetry Operations

(1) \(1\) 1\( \in \in \) 1

(2) 2' 0,0,z
(2'z 0,0,0)

(3) 4' 0,0,z
(4'z 0,0,0)

(4) 4' 0,0,z
(4'z 0,0,0)

(5) 2' 0,y,0
(2'y 0,0,0)

(6) 2' x,0,0
(2'x 0,0,0)

(7) 2 x,x,0
(2xy 0,0,0)

(8) 2 x,x,0
(2xy 0,0,0)

(9) \(\bar{1}\) 0,0,0
(1 0,0,0)

(10) m x,y,0
(mx, 0,0,0)

(11) \(\bar{4}\) 0,0,z
(\(4\bar{z}\) 0,0,0)

(12) \(\bar{4}\) 0,0,z
(\(4\bar{z}\) 0,0,0)

(13) m' x,0,z
(m'x, 0,0,0)

(14) m' 0,y,z
(m'y, 0,0,0)

(15) m x,x,z
(mx, 0,0,0)

(16) m x,x,z
(mx, 0,0,0)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>16</td>
<td>u</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8</td>
<td>t</td>
<td>.m'</td>
<td>x,1/2,z [u,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>s</td>
<td>.m'</td>
<td>x,0,z [u,0,w]</td>
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<tr>
<td>8</td>
<td>r</td>
<td>..m</td>
<td>x,x,z [u,u,0]</td>
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<td>q</td>
<td>m..</td>
<td>x,y,1/2 [0,0,w]</td>
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<td>m..</td>
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<td>m2'm'</td>
<td>x,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>n</td>
<td>m2'm'</td>
<td>x,1/2,0 [0,0,w]</td>
</tr>
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2  e  mm'm'.  0,1/2,1/2 [0,0,w]  1/2,0,1/2 [0,0,\bar{w}]
1  d  4'/mm'm'  1/2,1/2,1/2 [0,0,0]
1  c  4'/mm'm'  1/2,1/2,0 [0,0,0]
1  b  4'/mm'm'  0,0,1/2 [0,0,0]
1  a  4'/mm'm'  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  
\( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0] p2'mm'  
\( \mathbf{a}^* = -\mathbf{c} \)  \( \mathbf{b}^* = \mathbf{b} \)  
Origin at x,0,0

Along [1,1,0] p2mm1'  
\( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \)  \( \mathbf{b}^* = \mathbf{c} \)  
Origin at x,x,0
Origin at center (4'/mmm')

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y$

Symmetry Operations:

1. $1$ $(1|0,0,0)$
2. $2$ $0,0,z$ $(2_z|0,0,0)$
3. $4'$ $0,0,z$ $(4_z|0,0,0)'$
4. $4'$ $0,0,z$ $(4_z|0,0,0)'$
5. $2$ $0,y,0$ $(2_y|0,0,0)$
6. $2$ $x,0,0$ $(2_x|0,0,0)$
7. $2'$ $x,x,0$ $(2_{xy}|0,0,0)'$
8. $2'$ $x,x,0$ $(2_{xy}|0,0,0)'$
9. $\overline{1}$ $0,0,0$ $(\overline{1}|0,0,0)$
10. $m$ $x,y,0$ $(m_x|0,0,0)$
11. $4''$ $0,0,z$ $(4_z|0,0,0)'$
12. $4''$ $0,0,z$ $(4_z|0,0,0)'$
13. $m$ $x,0,z$ $(m_x|0,0,0)$
14. $m$ $0,y,z$ $(m_y|0,0,0)$
15. $m'$ $x,x,z$ $(m_{xy}|0,0,0)'$
16. $m'$ $x,x,z$ $(m_{xy}|0,0,0)'$

123.5.1003 - 1 - 2007
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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Symmetry of Special Projections

Along \([0,0,1]\) \(p4mm'\)  
\[a^* = a \quad b^* = b\]
Origin at 0,0,z

Along \([1,0,0]\) \(p2mm'\)  
\[a^* = b \quad b^* = c\]
Origin at x,0,0

Along \([1,1,0]\) \(p2'mm'\)  
\[a^* = -c \quad b^* = (-a + b)/2\]
Origin at x,x,0

2 e mmm. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]
1 d 4'/mmm' 1/2,1/2,1/2 [0,0,0]
1 c 4'/mmm' 1/2,1/2,0 [0,0,0]
1 b 4'/mmm' 0,0,1/2 [0,0,0]
1 a 4'/mmm' 0,0,0 [0,0,0]
Origin at center (4'/m'm'm)

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(3) 4' 0,0,z
(4z|0,0,0)'

(4) 4' 0,0,z
(4z|0,0,0)'

(5) 2 0,y,0
(2y|0,0,0)

(6) 2 x,0,0
(2x|0,0,0)

(7) 2' x,x,0
(2xy|0,0,0)'

(8) 2' x,x,0
(2xy|0,0,0)'

(9) T' 0,0,0
(1|0,0,0)'

(10) m' x,y,0
(mz|0,0,0)'

(11) 4' 0,0,z; 0,0,0
(4z|0,0,0)

(12) 4' 0,0,z; 0,0,0
(4z|0,0,0)

(13) m' x,0,z
(mx|0,0,0)'

(14) m' 0,y,z
(mx|0,0,0)'

(15) m x,x,z
(mxy|0,0,0)

(16) m x,x,z
(mxy|0,0,0)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Continued 123.6.1004 P4'/m'm'm

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Continued 123.6.1004 P4'/m'm'm

123.6.1004 - 2 - 2011
Symmetry of Special Projections

Along \([0,0,1]\) \(p4\)'m'm'\n\(a^* = a\) \(b^* = b\)
Origin at 0,0,z

Along \([1,0,0]\) \(p2\)'m'm'
\(a^* = b\) \(b^* = c\)
Origin at x,0,0

Along \([1,1,0]\) \(p2mm1'\)
\(a^* = (-a + b)/2\) \(b^* = c\)
Origin at x,x,0
Origin at center (4/mm'm')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \cdot 0,0,z \quad (2_z \cdot 0,0,0) \\
(3) & \quad 4^+ \cdot 0,0,z \quad (4_z \cdot 0,0,0) \\
(4) & \quad 4^- \cdot 0,0,z \quad (4_z^- \cdot 0,0,0) \\
(5) & \quad 2' \cdot 0,y,0 \quad (2_y \cdot 0,0,0)' \\
(6) & \quad 2' \cdot x,0,0 \quad (2_x \cdot 0,0,0)' \\
(7) & \quad 2' \cdot x,x,0 \quad (2_{xx} \cdot 0,0,0)' \\
(8) & \quad 2' \cdot x,x,0 \quad (2_{xx} \cdot 0,0,0)' \\
(9) & \quad \bar{1} \cdot 0,0,0 \\
(10) & \quad m \cdot x,y,0 \quad (m_y \cdot 0,0,0) \\
(11) & \quad \bar{4}^+ \cdot 0,0,z; 0,0,0 \quad (\bar{4}_z \cdot 0,0,0) \\
(12) & \quad \bar{4}^- \cdot 0,0,z; 0,0,0 \quad (\bar{4}_z^- \cdot 0,0,0) \\
(13) & \quad m' \cdot x,0,z \quad (m_y \cdot 0,0,0)' \\
(14) & \quad m' \cdot 0,y,z \quad (m_y \cdot 0,0,0)' \\
(15) & \quad m' \cdot x,x,z \quad (m_{xy} \cdot 0,0,0)' \\
(16) & \quad m' \cdot x,x,z \quad (m_{xy} \cdot 0,0,0)' 
\end{align*}
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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<td>2</td>
<td>f</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Origin at x,0,0</th>
<th>Origin at x,x,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4mm1'</td>
<td>p2'mm'</td>
</tr>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = -c b* = b</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2'mm'</td>
<td>p2'mm'</td>
</tr>
<tr>
<td>a* = -c b* = b</td>
<td>a* = -c b* = (-a + b)/2</td>
<td></td>
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<tr>
<td>Along [1,1,0]</td>
<td>p2'mm'</td>
<td></td>
</tr>
<tr>
<td>a* = -c b* = (-a + b)/2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (4'/m'2/m')

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x < y

Symmetry Operations

1. 1
   (1 | 0,0,0)

2. 2' 0,0,z
   (2 | z,0,0,0)

3. 4' 0,0,z
   (4 | z,0,0,0)'

4. 4' - 0,0,z
   (4 | z,0,0,0)'

5. 2' 0,y,0
   (2 | y,0,0,0)'

6. 2' x,0,0
   (2 | x,0,0,0)'

7. 2 x,x,0
   (2 | x,0,0,0)'

8. 2 x,x,0
   (2 | x,0,0,0)'

9. 1' 0,0,0
   (1 | 0,0,0)'

10. m' x,y,0
    (m | x,y,0)'

11. 4' + 0,0,z; 0,0,0
    (4 | z,0,0,0)'

12. 4' + 0,0,z; 0,0,0
    (4 | z,0,0,0)'

13. m x,0,z
    (m | 0,0,0)

14. m 0,y,z
    (m | 0,0,0)'

15. m' x,x,z
    (m | 0,0,0)'

16. m' x,x,z
    (m | 0,0,0)'

P4'/m'm'm'
123.8.1006
4'/m'm'm'
P4'/m'2/m2/m'

Tetragonal
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<td></td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<td>(10) x,y,z [u,v,w]</td>
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<td>x,y,1/2 [u,v,0]</td>
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<td>o</td>
<td>m'2m. x,1/2,1/2 [0,v,0]</td>
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<td>x,1/2,1/2 [0,v,0]</td>
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<td>x,0,0 [0,v,0]</td>
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<td>x,0,0 [0,v,0]</td>
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<tr>
<td>4</td>
<td>k</td>
<td>m'.2m' x,x,1/2 [u,u,0]</td>
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<td>x,x,1/2 [u,u,0]</td>
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<td>x,x,1/2 [u,u,0]</td>
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<td>j</td>
<td>m'.2m' x,x,0 [u,u,0]</td>
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<td>x,x,0 [u,u,0]</td>
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<td>x,x,0 [u,u,0]</td>
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<td>2mm. 0,1/2,z [0,0,0]</td>
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<td>0,1/2,z [0,0,0]</td>
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<td>1/2,0,0 [0,0,0]</td>
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<td>1/2,0,0 [0,0,0]</td>
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<tr>
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<td>h</td>
<td>4'mm' 1/2,1/2,z [0,0,0]</td>
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<td>1/2,1/2,z [0,0,0]</td>
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<tr>
<td>2</td>
<td>g</td>
<td>4'mm' 0,0,z [0,0,0]</td>
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<td>0,0,z [0,0,0]</td>
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<tr>
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<td>f</td>
<td>m'2m. 0,1/2,0 [0,0,0]</td>
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<tr>
<td></td>
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<td>1/2,0,0 [0,0,0]</td>
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</tbody>
</table>
Continued

Symmetry of Special Projections

Along \([0,0,1]\)  \(p4'm'm'\)  \(\mathbf{a}^* = \mathbf{a}\)  \(\mathbf{b}^* = \mathbf{b}\)  Origin at 0,0,z

Along \([1,0,0]\)  \(p2mm1'\)  \(\mathbf{a}^* = \mathbf{b}\)  \(\mathbf{b}^* = \mathbf{c}\)  Origin at x,0,0

Along \([1,1,0]\)  \(p2m'm'\)  \(\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2\)  \(\mathbf{b}^* = \mathbf{c}\)  Origin at x,x,0
P4/m'2/m'2/m'
123.9.1007
Tetragonal

Origin at center ( 4/m'2/m'2/m' )

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

Symmetry Operations

1. \( 1 \)
   \( (0,0,0) \)
2. \( 2 \)
   \( x,0,0 \)
3. \( 4 \)
   \( x,x,0 \)
4. \( 4 \)
   \( x,x,0 \)
5. \( 2 \)
   \( x,0,z \)
6. \( 2 \)
   \( x,0,z \)
7. \( 4 \)
   \( x,x,0 \)
8. \( 4 \)
   \( x,x,0 \)
9. \( 2 \)
   \( x,0,0 \)
10. \( 2 \)
    \( x,0,0 \)
11. \( 4 \)
    \( x,x,0 \)
12. \( 4 \)
    \( x,x,0 \)
13. \( m' \)
    \( x,0,z \)
14. \( m' \)
    \( x,0,z \)
15. \( m' \)
    \( x,x,z \)
16. \( m' \)
    \( x,x,z \)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>16 u 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(9) x,y,z [u,v,w] (10) x,y,z [u,v,w] (11) y,x,z [v,u,w] (12) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(13) x,y,z [u,v,w] (14) x,y,z [u,v,w] (15) y,x,z [v,u,w] (16) y,x,z [v,u,w]</td>
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</tr>
<tr>
<td>8 t .m'</td>
<td>x,1/2,z [u,0,w] x,1/2,z [u,0,w] 1/2,x,z [0,u,w] 1/2,x,z [0,u,w]</td>
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<tr>
<td>x,1/2,z [u,0,w] x,1/2,z [u,0,w] 1/2,x,z [0,u,w] 1/2,x,z [0,u,w]</td>
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<tr>
<td>8 s .m'</td>
<td>x,0,z [u,0,w] x,0,z [u,0,w] 0,x,z [0,u,w] 0,x,z [0,u,w]</td>
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<tr>
<td>x,0,z [u,0,w] x,0,z [u,0,w] 0,x,z [0,u,w] 0,x,z [0,u,w]</td>
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<td>8 r ..m'</td>
<td>x,x,z [u,u,w] x,x,z [u,u,w] x,x,z [u,u,w] x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w] x,x,z [u,u,w] x,x,z [u,u,w] x,x,z [u,u,w]</td>
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<tr>
<td>8 q m'..'</td>
<td>x,y,1/2 [u,v,0] x,y,1/2 [u,v,0] y,x,1/2 [v,u,0] y,x,1/2 [v,u,0]</td>
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<td>x,y,1/2 [u,v,0] x,y,1/2 [u,v,0] y,x,1/2 [v,u,0] y,x,1/2 [v,u,0]</td>
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<tr>
<td>8 p m'..'</td>
<td>x,y,0 [u,v,0] x,y,0 [u,v,0] y,x,0 [v,u,0] y,x,0 [v,u,0]</td>
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<td>x,y,0 [u,v,0] x,y,0 [u,v,0] y,x,0 [v,u,0] y,x,0 [v,u,0]</td>
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<tr>
<td>4 o m'2m'</td>
<td>x,1/2,1/2 [u,0,0] x,1/2,1/2 [u,0,0] 1/2,x,1/2 [0,u,0] 1/2,x,1/2 [0,u,0]</td>
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<td>x,1/2,1/2 [u,0,0] x,1/2,1/2 [u,0,0] 1/2,x,1/2 [0,u,0] 1/2,x,1/2 [0,u,0]</td>
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<tr>
<td>4 n m'2m'</td>
<td>x,1/2,0 [u,0,0] x,1/2,0 [u,0,0] 1/2,x,0 [0,u,0] 1/2,x,0 [0,u,0]</td>
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<tr>
<td>4 l m'2m'</td>
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<td>x,0,0 [u,0,0] x,0,0 [u,0,0] 0,x,0 [0,u,0] 0,x,0 [0,u,0]</td>
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<tr>
<td>4 k m'2m'</td>
<td>x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0]</td>
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<td>4 j m'2m'</td>
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<tr>
<td>4 i 2m'</td>
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<tr>
<td>1</td>
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<tr>
<td>1</td>
<td>b</td>
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<tr>
<td>1</td>
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**Symmetry of Special Projections**

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<tr>
<th>Along [0,0,1]</th>
<th>p4m\textquotesingle m\textquotesingle</th>
<th>Along [1,0,0]</th>
<th>p2m\textquotesingle m\textquotesingle</th>
<th>Along [1,1,0]</th>
<th>p2m\textquotesingle m\textquotesingle</th>
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<tr>
<td>(a^* = a) (b^* = b)</td>
<td>(a^* = b) (b^* = c)</td>
<td>(a^* = (-a + b)/2) (b^* = c)</td>
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<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
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### Origin

At center (4/mmm)

### Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

### Symmetry Operations

**For \((0,0,0)\) + set**

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<td>(1)</td>
<td>( 0,0,0 )</td>
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<tr>
<td>(2)</td>
<td>( 2 )</td>
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<tr>
<td>(2)</td>
<td>( 0,0,z )</td>
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<td>(3)</td>
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<td>(3)</td>
<td>( 0,0,z )</td>
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<td>(4)</td>
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<td>( 0,0,z )</td>
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</table>

**For \((0,0,1)\)' + set**

<table>
<thead>
<tr>
<th>Number</th>
<th>Symmetry Operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>( t'(0,0,1) )</td>
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<tr>
<td>(1)</td>
<td>( 0,0,1 )</td>
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<tr>
<td>(2)</td>
<td>( 2'(0,0,1) )</td>
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<td>( 4^+ )</td>
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<td>(3)</td>
<td>( (0,0,1) )</td>
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<td>( 4 )</td>
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<td>( 0,0,z )</td>
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<td>( 0,0,z )</td>
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### Generators selected

\((1), \{(0,1,0)\}; \{(0,0,1)\}; \{t'(0,0,1)\}; (2); (3); (5); (9)\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td></td>
<td>((0,0,0)) +</td>
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<tr>
<td>32 u 1</td>
<td>(x,y,z) [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(\bar{x},\bar{y},\bar{z}) [u,v,w]</td>
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<tr>
<td>16 t.m.</td>
<td>(x,1/2,z) [0,v,0]</td>
</tr>
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<td>(\bar{x},1/2,\bar{z}) [0,v,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [1,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>

16 s .m. x,0,z [0,v,0] x,0,z [0,v,0] 0,x,z [v,0,0] 0,x,z [v,0,0] 16 r .m. x,x,z [u,u,0] x,x,z [u,u,0] x,x,z [u,u,0] 16 q m.. x,y,1/2 [u,v,0] x,y,1/2 [u,v,0] y,x,1/2 [v,u,0] y,x,1/2 [v,u,0] 16 p m.. x,y,0 [0,0,w] x,y,0 [0,0,w] y,x,0 [0,0,w] y,x,0 [0,0,w] 8 o m'2'm. x,1/2,1/2 [0,v,0] 1/2,x,1/2 [v,0,0] 1/2,x,1/2 [v,0,0] 8 n m2m. x,1/2,0 [0,0,0] 1/2,x,0 [0,0,0] 1/2,x,0 [0,0,0] 8 m m'2'm. x,0,1/2 [0,v,0] 0,x,1/2 [v,0,0] 0,x,1/2 [v,0,0] 8 l m2m. x,0,0 [0,0,0] 0,x,0 [0,0,0] 0,x,0 [0,0,0] 8 k m'.2'm x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] 8 j m.2m x,x,0 [0,0,0] x,x,0 [0,0,0] x,x,0 [0,0,0] x,x,0 [0,0,0] 8 i 2mm. 0,1/2,z [0,0,0] 1/2,0,z [0,0,0] 1/2,0,z [0,0,0] 4 h 4mm 1/2,1/2,z [0,0,0] 1/2,1/2,z [0,0,0] 1/2,1/2,z [0,0,0] 4 g 4mm 0,0,z [0,0,0] 0,0,z [0,0,0] 0,0,z [0,0,0] 4 f mmm. 0,1/2,0 [0,0,0] 1/2,0,0 [0,0,0] 1/2,0,0 [0,0,0] 4 e m'mm. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 2 d 4/m'mm 1/2,1/2,1/2 [0,0,0] 2 c 4/mmm 1/2,1/2,0 [0,0,0] 2 b 4/m'mm 0,0,1/2 [0,0,0] 2 a 4/mmm 0,0,0 [0,0,0]
Origin at center (4/mmm)

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(3) 4+ 0,0,z
(4z|0,0,0)

(4) 4− 0,0,z
(4z−1|0,0,0)

(5) 2 0,y,0
(2y|0,0,0)

(6) 2 x,0,0
(2x|0,0,0)

(7) 2 x,0,x
(2yx|0,0,0)

(8) 2 x,x,0
(2xy|0,0,0)

(9) m 0,0,0
(m|0,0,0)

(10) m x,y,0
(mx|0,0,0)

(11) 4+ 0,0,z; 0,0,0
(4z|0,0,0)

(12) 4− 0,0,z; 0,0,0
(4z−1|0,0,0)

(13) m x,0,z
(mx|0,0,0)

(14) m 0,y,z
(mx|0,0,0)

(15) m x,x,z
(mx|0,0,0)

(16) m x,x,z
(mx|0,0,0)
For (1,0,0)' + set

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>(1) t' (1,0,0)</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>(1</td>
<td>1,0,0)'</td>
</tr>
<tr>
<td>(2) 2' 1/2,0,z</td>
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</tr>
<tr>
<td>(2</td>
<td>1,0,0)'</td>
</tr>
<tr>
<td>(3) 4' -1/2,1/2,z</td>
<td></td>
</tr>
<tr>
<td>(4</td>
<td>1,0,0)'</td>
</tr>
<tr>
<td>(4' 1/2,-1/2,z</td>
<td></td>
</tr>
<tr>
<td>(4'</td>
<td>1,0,0)'</td>
</tr>
<tr>
<td>(5) 2' 1/2,y,0</td>
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<td>1,0,0)'</td>
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<td>(6) 2' (1,0,0)</td>
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<td>(7) 2' (1/2,1/2,0)</td>
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<td>(8) 2' (1/2,-1/2,0)</td>
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<tr>
<td>(9) T' 1/2,0,0</td>
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<tr>
<td>(1) t' (1,0,0)</td>
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<td>(10) a' (1,0,0)</td>
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<td>(m</td>
<td>1,0,0)'</td>
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<td>(11) 4' 1/2,-1/2,z</td>
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<td>(1/2,1,0,0)'</td>
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<td>(12) 4' 1/2,1/2,0</td>
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<td>(1/2,1,0,0)'</td>
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<td>(13) a' (1,0,0)</td>
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<td>(m</td>
<td>1,0,0)'</td>
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<td>(14) m' 1/2,y,z</td>
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<td>(m</td>
<td>1,0,0)'</td>
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<td>(15) g' (1/2,-1/2,0)</td>
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<td>(1/2,1,0,0)'</td>
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<td>(16) g' (1/2,1/2,0)</td>
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<td>(1/2,1,0,0)'</td>
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Positions selected (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
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</table>
8  l  m2m.  x,0,0 [0,0,0]  \bar{x},0,0 [0,0,0]  0,x,0 [0,0,0]  0,\bar{x},0 [0,0,0]
8  k  m.2m  x,x,1/2 [0,0,0]  \bar{x},x,1/2 [0,0,0]  x,x,1/2 [0,0,0]  x,\bar{x},1/2 [0,0,0]
8  j  m.2m  x,x,0 [0,0,0]  \bar{x},x,0 [0,0,0]  x,x,0 [0,0,0]  x,\bar{x},0 [0,0,0]
8  i  2'nm'.  0,1/2,z [u,0,0]  1/2,0,z [u,0,0]  0,1/2,\bar{z} [u,0,0]  1/2,0,\bar{z} [u,0,0]
4  h  4'm'm  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]
4  g  4mm  0,0,z [0,0,0]  0,0,\bar{z} [0,0,0]
4  f  mm'.  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]
4  e  mm'.  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]
2  d  4'/mm'm  1/2,1/2,1/2 [0,0,0]
2  c  4'/mm'm  1/2,1/2,0 [0,0,0]
2  b  4mmm  0,0,1/2 [0,0,0]
2  a  4/mmm  0,0,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  p4mm1'  a' = a  b' = b  Origin at 0,0,z
Along [1,0,0]  p2mm1'  a' = b  b' = c  Origin at x,0,0
Along [1,1,0]  p2mm1'  a' = (-a + b)/2  b' = c  Origin at x,x,0
PI 4/mmm
123.12.1010

4/mmm1'
P_4/m2/m2/m

Tetragonal
**Origin** at center (4/mmm)

**Asymmetric unit**  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

**Symmetry Operations**

For \((0,0,0)\) + set

1. \((1)\) \(1\)  
   \((1|0,0,0)\)  
2. \((2)\) \(2\) \(0,0,z\)  
   \((2z|0,0,0)\)  
3. \((3)\) \(4^+\) \(0,0,z\)  
   \((4z|0,0,0)\)  
4. \((4)\) \(4^-\) \(0,0,z\)  
   \((4z^-|0,0,0)\)

5. \((5)\) \(2\) \(0,y,0\)  
   \((2z|0,0,0)\)

9. \((9)\) \(\overline{1}\) \(0,0,0\)  
   \((1\overline{1}|0,0,0)\)

13. \((13)\) \(m\) \(x,0,z\)  
   \((m_\parallel|0,0,0)\)

For \((1,0,0)\)' + set

1. \((1)\) \(t'\) \((1,0,0)\)  
   \((1,0,0)'\)

5. \((5)\) \(2'\) \(1/2,y,0\)  
   \((2z|1,0,0)'\)

9. \((9)\) \(\overline{1}\) \(1/2,0,0\)  
   \((\overline{1}|1,0,0)'\)

13. \((13)\) \(a'\) \((1,0,0)\) \(x,0,z\)  
   \((m_\parallel|1,0,0)'\)

Generators selected  
1. \(t'(1,0,0)\); \(t'(0,1,0)\); \(t'(0,0,1)\); \((2)\); \((3)\); \((5)\); \((9)\).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>((0,0,0) + )</th>
<th>((1,0,0)' + )</th>
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</thead>
<tbody>
<tr>
<td>(32) (u) 1</td>
<td>(1) (x,y,z) ([u,v,w])</td>
<td>(2) (\overline{x},\overline{y},\overline{z}) ([u,\overline{v},w])</td>
</tr>
<tr>
<td></td>
<td>(5) (x,y,\overline{z}) ([u,\overline{v},w])</td>
<td>(6) (x,\overline{y},\overline{z}) ([u,\overline{v},\overline{w}])</td>
</tr>
<tr>
<td></td>
<td>(9) (\overline{x},\overline{y},\overline{z}) ([u,\overline{v},w])</td>
<td>(10) (x,y,\overline{z}) ([u,\overline{v},w])</td>
</tr>
<tr>
<td></td>
<td>(13) (x,y,\overline{z}) ([u,\overline{v},w])</td>
<td>(14) (x,\overline{y},\overline{z}) ([u,\overline{v},w])</td>
</tr>
<tr>
<td>(16) (t) (m')</td>
<td>(x,1/2,z) ([u,0,w])</td>
<td>(\overline{x},1/2,z) ([\overline{u},0,w])</td>
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</table>
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Transformation</th>
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</thead>
<tbody>
<tr>
<td>s</td>
<td>m..</td>
<td>x,0,z [0,v,0]</td>
</tr>
<tr>
<td>r</td>
<td>..m</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>q</td>
<td>m'..</td>
<td>x,y,1/2 [u,v,0]</td>
</tr>
<tr>
<td>p</td>
<td>m..</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td>o</td>
<td>m'2m'</td>
<td>x,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>n</td>
<td>m2m'</td>
<td>x,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>m</td>
<td>m'2m'</td>
<td>x,0,1/2 [0,v,0]</td>
</tr>
<tr>
<td>l</td>
<td>m2m</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>k</td>
<td>m'.2'm</td>
<td>x,x,1/2 [u,u,0]</td>
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<td>j</td>
<td>m.2m</td>
<td>x,x,0 [0,0,0]</td>
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<td>i</td>
<td>2'mm'</td>
<td>0,1/2,z [u,0,0]</td>
</tr>
<tr>
<td>h</td>
<td>4'm'm</td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>g</td>
<td>4mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>f</td>
<td>mm'm</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>e</td>
<td>m'm'm'</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>d</td>
<td>4'/m'm'm</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>c</td>
<td>4'/mm'm</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>b</td>
<td>4'm'mm</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>a</td>
<td>4'mmm</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Along [0,0,1] p4mm1'  
\[ a^* = a \quad b^* = b \]  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\[ a^* = b \quad b^* = c \]  
Origin at x,0,0

Along [1,1,0] p2mm1'  
\[ a^* = (-a + b)/2 \quad b^* = c \]  
Origin at x,x,0
P_2c 4'/mm'1'  
123.13.1011  
P_2c 4'/m2'/m'2/m 

Tetragonal
Origin at center (4/mmm)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

For (0,0,0) + set

1. 1
   (1 0 0 0)

2. 2 0 0, z
   (2z 0 0, 0)

3. 4* 0 0, z
   (4z 0 0, 0)

4. 4* 0 0, z
   (4z 0 0, 0)

5. 2' 0, y, 0
   (2z 0 0, 0)

6. 2' x, 0, 0
   (2z 0 0, 0)

7. 2 x, x, 0
   (2xy 0 0, 0)

8. 2 x, x, 0
   (2xy 0 0, 0)

9. T 0, 0, 0
   (0 0 0)

10. m x, y, 0
    (mz 0 0, 0)

11. 4 + 0, 0, z; 0, 0, 0
    (4z 0 0, 0)

12. 4 + 0, 0, z; 0, 0, 0
    (4z 0 0, 0)

13. m' x, 0, z
    (m'z 0 0, 0)

14. m' 0, y, z
    (mz 0 0, 0)

15. m x, x, z
    (mx 0 0, 0)

16. m x, x, z
    (mx 0 0, 0)

For (0,0,1) + set

1. t 0, 0, 1
   (1 0 0, 1)

2. 2' 0, 0, 1
   (2z 0 0, 0)

3. 4* 0, 0, 1
   (4z 0 0, 1)

4. 4* 0, 0, 1
   (4z 0 0, 1)

5. 2 0, y, 1/2
   (2z 0 0, 0)

6. 2 x, 0, 1/2
   (2z 0 0, 0)

7. 2 x, x, 1/2
   (2xy 0 0, 1)

8. 2 x, x, 1/2
   (2xy 0 0, 1)

9. T 0, 0, 1/2
   (0 0 1)

10. m'' x, y, 1/2
    (mz 0 0, 1)

11. 4 + 0, 0, z; 0, 0, 1/2
    (4z 0 0, 1)

12. 4 + 0, 0, z; 0, 0, 1/2
    (4z 0 0, 1)

13. c 0, 0, 1
    (mz 0 0, 1)

14. c 0, 0, 1
    (mz 0 0, 1)

15. c' 0, 0, 1
    (mxz 0 0, 1)

16. c' 0, 0, 1
    (mxz 0 0, 1)

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
<th>Multiplicity</th>
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<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>32 u 1</td>
<td>(0,0,0) +</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(0,0,1)' +</td>
<td>(0,0,1)' +</td>
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</tbody>
</table>

32 u 1
(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y,x,z [v,u,w]  (4) y,x,z [v,u,w]
(5) x,y,z [u,v,w]  (6) x,y,z [u,v,w]  (7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]
(9) x,y,z [u,v,w]  (10) x,y,z [u,v,w]  (11) y,x,z [v,u,w]  (12) y,x,z [v,u,w]
(13) x,y,z [u,v,w]  (14) x,y,z [u,v,w]  (15) y,x,z [v,u,w]  (16) y,x,z [v,u,w]

16 t .m'
(1) x,1/2,z [u,0,w]  (2) x,1/2,z [u,0,w]  (3) x,1/2,z [u,0,w]  (4) x,1/2,z [u,0,w]
(5) x,1/2,z [u,0,w]  (6) x,1/2,z [u,0,w]  (7) x,1/2,z [u,0,w]  (8) x,1/2,z [u,0,w]
| 16 s | .m' | x,0,z [u,0,w] | x,0,z [u,0,w] | 0,x,z [0,u,w] | 0,x,z [0,u,w] | 0,x,z [0,u,w] |
| 16 r | .m | x,x,z [u,u,0] | x,x,z [u,u,0] | x,x,z [u,u,0] | x,x,z [u,u,0] |
| 16 q | m' | x,y,1/2 [u,v,0] | x,y,1/2 [u,v,0] | y,x,1/2 [v,u,0] | y,x,1/2 [v,u,0] |
| 16 p | m | x,y,0 [0,0,w] | x,y,0 [0,0,w] | y,x,0 [0,0,w] | y,x,0 [0,0,w] |
| 8 o | m'2m' | x,1/2,1/2 [u,0,0] | x,1/2,1/2 [u,0,0] | 1/2,x,1/2 [0,u,0] | 1/2,x,1/2 [0,u,0] |
| 8 n | m'2m' | x,1/2,0 [0,0,w] | x,1/2,0 [0,0,w] | 1/2,x,0 [0,0,w] | 1/2,x,0 [0,0,w] |
| 8 m | m'2m' | x,0,1/2 [u,0,0] | x,0,1/2 [u,0,0] | 0,x,1/2 [0,u,0] | 0,x,1/2 [0,u,0] |
| 8 l | m2m' | x,0,0 [0,0,w] | x,0,0 [0,0,w] | 0,x,0 [0,0,w] | 0,x,0 [0,0,w] |
| 8 k | m'.2m | x,x,1/2 [u,u,0] | x,x,1/2 [u,u,0] | x,x,1/2 [u,u,0] | x,x,1/2 [u,u,0] |
| 8 j | m.2m | x,x,0 [0,0,w] | x,x,0 [0,0,w] | x,x,0 [0,0,w] | x,x,0 [0,0,w] |
| 8 i | 2m'm' | 0,1/2,z [0,0,0] | 0,1/2,z [0,0,0] | 0,1/2,z [0,0,0] | 0,1/2,z [0,0,0] |
| 4 h | 4'm'm | 1/2,1/2,z [0,0,0] | 1/2,1/2,z [0,0,0] | 1/2,1/2,z [0,0,0] |
| 4 g | 4'm'm | 0,0,z [0,0,0] | 0,0,z [0,0,0] |
| 4 f | mm'm'. | 0,1/2,0 [0,0,w] | 1/2,0,0 [0,0,w] |
| 4 e | m'mm. | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |
| 2 d | 4'/m'm'm | 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |
| 2 c | 4'/mm'm | 1/2,1/2,0 [0,0,0] |
| 2 b | 4'/mm'm | 0,0,1/2 [0,0,0] |
| 2 a | 4'/mm'm | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

| Along [0,0,1] | p4mm1' | a* = a | b* = b |
| Along [1,0,0] | p2mm' | a* = -c | b* = b |
| Along [1,1,0] | p2mm1' | a* = (-a + b)/2 | b* = c |

Origin at 0,0,z

Origin at x,0,0

Origin at x,x,0
P_2c'4'/mmm'
123.14.1012

4/mmm1'
P_2c'4'/m2/m2'/m'

Tetragonal
Origin at center (4'/mmm')

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

For (0,0,0) + set

<table>
<thead>
<tr>
<th>(1) 1</th>
<th>(2) 2  x,y,z</th>
<th>(3) 4' x,y,z</th>
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<td>(1,0,0)</td>
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<th>(9) 1</th>
<th>(10) m 0,1/2</th>
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For (0,0,1)' + set

<table>
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<tr>
<th>(1) t</th>
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Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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Continued 123.14.1012 P 2c 4'/mmm'

Origin at center (4'/mmm')

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

For (0,0,0) + set

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Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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123.14.1012 - 2 - 2035
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<tr>
<td>4</td>
<td>g</td>
<td>4'mm'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<tr>
<td>4</td>
<td>f</td>
<td>mmm.</td>
<td>0,1/2,0 [0,0,0]</td>
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<tr>
<td>4</td>
<td>e</td>
<td>m'mm.</td>
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<tr>
<td>2</td>
<td>d</td>
<td>4'/m'mm'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2</td>
<td>c</td>
<td>4'/m'mm'</td>
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<tr>
<td>2</td>
<td>b</td>
<td>4'/m'mm'</td>
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<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2</td>
<td>a</td>
<td>4'/mmm'</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [1,1,0]</th>
<th>p2a* 2'mm'</th>
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<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = -c</td>
<td>b* = (-a + b)/2</td>
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<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
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</table>
P$_{2c}$ 4/mmm$^1$

123.15.1013

P$_{2c}$ 4/m2'/m'2'/m'

4/mmm$^1$

Tetragonal
Origin at center (4/mm'm')

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(3) 4* 0,0,z
(4z|0,0,0)

(4) 4* 0,0,0
(4z'|0,0,0)

(5) 2' 0,y,0
(2z|0,0,0)

(6) 2' x,0,0
(2z|0,0,0)

(7) 2' x,x,0
(2z|0,0,0)

(8) 2' x,x,0
(2y|0,0,0)

(9) T 0,0,0
(T|0,0,0)

(10) m x,y,0
(m|x,0,0)

(11) 4* 0,0,z; 0,0,0
(4z|0,0,0)

(12) 4* 0,0,z; 0,0,0
(4z'|0,0,0)

(13) m' x,0,z
(m'|0,0,0)

For (0,0,1)' + set

(1) t'(0,0,1)
(1|0,0,1)'

(2) 2' (0,0,1) 0,0,z
(2z|0,0,1)'

(3) 4* '(0,0,1) 0,0,z
(4z|0,0,1)'

(4) 4* '(0,0,1) 0,0,0
(4z'|0,0,1)'

(5) 2 0,y,1/2
(2z|0,0,1)

(6) 2 x,0,1/2
(2z|0,0,1)

(7) 2 x,x,1/2
(2z|0,0,1)

(8) 2 x,x,1/2
(2y|0,0,1)

(9) T 0,0,1/2
(T|0,0,1)'

(10) m' x,y,1/2
(m'|0,0,1)'

(11) 4* x,0,z; 0,0,1/2
(4z|0,0,1)'

(12) 4* x,0,z; 0,0,1/2
(4z'|0,0,1)'

(13) c (0,0,1) x,0,z
(m|0,0,1)

(14) c (0,0,1) 0,y,z
(m|0,0,1)

(15) c (0,0,1) x,x,0
(mxy|0,0,1)

(16) c (0,0,1) x,x,0
(mxy|0,0,1)

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

(0,0,0) +  (0,0,1)' +

32  u  1  (1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y,x,z [v,u,w]  (4) y,x,z [v,u,w]

(5) x,y,z [u,v,w]  (6) x,y,z [u,v,w]  (7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]

(9) x,y,z [u,v,w]  (10) x,y,z [u,v,w]  (11) y,x,z [v,u,w]  (12) y,x,z [v,u,w]

(13) x,y,z [u,v,w]  (14) x,y,z [u,v,w]  (15) y,x,z [v,u,w]  (16) y,x,z [v,u,w]

16  t .m'  x,1/2,z [u,0,w]  x,1/2,z [u,0,w]  1/2,x,z [0,u,w]  1/2,x,z [0,u,w]

x,1/2,z [u,0,w]  x,1/2,z [u,0,w]  1/2,x,z [0,u,w]  1/2,x,z [0,u,w]
Symmetry of Special Projections

Along \([0,0,1]\)  \(p4mm1'\)

\(a^* = a\) \(b^* = b\)

Origin at 0,0,z

Along \([1,0,0]\)  \(p_2a^-2'nm'\)

\(a^* = -c\) \(b^* = b\)

Origin at x,0,0

Along \([1,1,0]\)  \(p_2a^-2'nm'\)

\(a^* = -c\) \(b^* = (-a + b)/2\)

Origin at x,x,0

\(\)
Origin at center (4/m'mm)

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x < y

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1) 0,0,0
(5) 2' 0,y,0
    (2) 0,0,z
    (2) 0,0,0
    (2) 0,0,0
(9) T' 0,0,0
    (3) 4', 0,0,z
    (3) 0,0,0
    (4) 0,0,0
    (4) 0,0,0
(13) m x,0,z
    (m) x,0,0
    (m) x,0,0
    (m) x,0,0
(17) m x,0,0
    (m) x,0,0
    (m) x,0,0
    (m) x,0,0
For (1,0,0)' + set

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<thead>
<tr>
<th>Precise Coordinates</th>
<th>Wyckoff letter, Multiplicity, Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t' (1,0,0)</td>
<td>(123.16.1014)</td>
</tr>
<tr>
<td>(2') 1/2,0,z</td>
<td>(4') -1/2,1/2,z</td>
</tr>
<tr>
<td>(2') 1/2,0,z</td>
<td>(4') -1/2,1/2,z</td>
</tr>
<tr>
<td>(3) 4' -1/2,1/2,z</td>
<td>(4) 1/2,1/2,z</td>
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<tr>
<td>(4) 1/2,1/2,z</td>
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</tr>
<tr>
<td>(5) 2 1/2,y,0</td>
<td>(2) 1/2,1/2,0</td>
</tr>
<tr>
<td>(2) 1/2,1/2,0</td>
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</tr>
<tr>
<td>(6) 2 1/2,1/2,0</td>
<td></td>
</tr>
<tr>
<td>(7) 2 1/2,1/2,0</td>
<td></td>
</tr>
<tr>
<td>(8) 2 1/2,1/2,0</td>
<td></td>
</tr>
<tr>
<td>(9) T 1/2,0,0</td>
<td>(13) a' (1,0,0)</td>
</tr>
<tr>
<td>(10) a' (1,0,0)</td>
<td>(14) m' 1/2,y,z</td>
</tr>
<tr>
<td>(11) 4' 1/2,1/2,z</td>
<td>(15) g' (1/2,1/2,0)</td>
</tr>
<tr>
<td>(12) 4' 1/2,1/2,z</td>
<td>(16) g' (1/2,1/2,0)</td>
</tr>
<tr>
<td>(13) a' (1,0,0)</td>
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</tr>
<tr>
<td>(14) m' 1/2,y,z</td>
<td></td>
</tr>
<tr>
<td>(15) g' (1/2,1/2,0)</td>
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</tr>
<tr>
<td>(16) g' (1/2,1/2,0)</td>
<td></td>
</tr>
</tbody>
</table>

Generators selected (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Coordinates</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
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</tr>
<tr>
<td>32 u 1</td>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>16 t .m'.</td>
<td>(2) x',y,z</td>
<td>[u',v,w]</td>
</tr>
<tr>
<td>16 s .m.</td>
<td>(3) y',x,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>16 r ..m</td>
<td>(4) y,x,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>16 q m'..</td>
<td>(5) x,y,1/2</td>
<td>[u,v,0]</td>
</tr>
<tr>
<td>16 p m'..</td>
<td>(6) x,y,1/2</td>
<td>[u,v,0]</td>
</tr>
<tr>
<td>8 o m'2m'.</td>
<td>(7) x,1/2,1/2</td>
<td>[u,0,0]</td>
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<tr>
<td>8 n m'2m'.</td>
<td>(8) x,1/2,0</td>
<td>[u,0,0]</td>
</tr>
<tr>
<td>8 m m'2m'.</td>
<td>(9) x,0,1/2</td>
<td>[0,v,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p\_p 4mm
\textbf{a}^* = a \quad \textbf{b}^* = \textbf{b} \\
Origin at 0,0,z

Along [1,0,0] p2mm1'
\textbf{a}^* = \textbf{b} \quad \textbf{b}^* = c \\
Origin at x,0,0

Along [1,1,0] p2mm1'
\textbf{a}^* = (-\textbf{a} + \textbf{b})/2 \quad \textbf{b}^* = c \\
Origin at x,x,0
Origin at center (4'/mmm')

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \quad (1|0,0,0) \\
(5) & \quad 2 \quad 0,y,0 \quad (2z|0,0,0) \\
(9) & \quad \bar{1} \quad 0,0,0 \quad (1|0,0,0) \\
(13) & \quad m \quad x,0,z \quad (mz|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \quad (2z|0,0,0) \\
(6) & \quad 2 \quad x,0,0 \quad (2z|x,0,0) \\
(10) & \quad m \quad x,y,0 \quad (mz|x,0,0) \\
(3) & \quad 4^{+} \quad 0,0,z \quad (4z|0,0,0) \quad (4z^{-1}|0,0,0)' \\
(7) & \quad 2' \quad x,x,0 \quad (2x|x,0,0) \quad (2x^{-1}|0,0,0)' \\
(11) & \quad \bar{4}^{+} \quad 0,0,z; 0,0,0 \quad (4z|0,0,0) \quad (4z^{-1}|0,0,0)' \\
(15) & \quad m' \quad x,x,z \quad (mz|0,0,0) \quad (mz^{-1}|0,0,0)' \\
(4) & \quad 4^{+} \quad 0,0,z \quad (4z|0,0,0) \quad (4z^{-1}|0,0,0)' \\
(8) & \quad 2' \quad x,x,0 \quad (2x|x,0,0) \quad (2x^{-1}|0,0,0)' \\
(12) & \quad \bar{4}^{+} \quad 0,0,z; 0,0,0 \quad (4z|0,0,0) \quad (4z^{-1}|0,0,0)' \\
(16) & \quad m' \quad x,x,z \quad (mz|0,0,0) \quad (mz^{-1}|0,0,0)' \\
\end{align*}
\]
For \((1,0,0)\)' + set

(1) \(t' (1,0,0)\)
(2) \(2' 1/2,0,z\)
(3) \(4' -1/2,1/2,z\)
(4) \(4' 1/2,-1/2,z\)

(5) \(2' 1/2,y,0\)
(6) \(2' (1,0,0) x,0,0\)
(7) \(2 (1/2,1/2,0) x+1/2,x,0\)
(8) \(2 (1/2,-1/2,0) x+1/2,x,0\)

(9) \(t (1,0,0)\)
(10) \(t (1,0,0)'\)
(11) \(4 1/2,-1/2,z; 1/2,1/2,z\)
(12) \(4 1/2,1/2,z; 1/2,1/2,z\)

(13) \(a' (1,0,0) x,0,z\)
(14) \(m' 1/2,y,z\)
(15) \(g (1/2,-1/2,0) x+1/2,x,0\)
(16) \(g (1/2,1/2,0) x+1/2,x,0\)

Generators selected \((1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9)\).

Positions

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<tr>
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<tr>
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<td>(x',y,z [u',v,w])</td>
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<td>(y',x,z [v,u,w])</td>
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<td>(4)</td>
<td>(y,x,z [v,u,w])</td>
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<td>x,1/2,z [u,0,w]</td>
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<td>x,1/2,z [u,0,w]</td>
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<td>(18)</td>
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<td>x,1/2,1/2 [0,0,w]</td>
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<td>(41)</td>
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\[\text{123.17.1015 - 2 - 2044}\]
Continued

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<tbody>
<tr>
<td>8</td>
<td>l</td>
<td>m2m. $x,0,0$ [0,0,0] $\bar{x},0,0$ [0,0,0] $0,x,0$ [0,0,0] $0,\bar{x},0$ [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>k</td>
<td>m.2'm' $x,x,1/2$ [0,0,w] $\bar{x},\bar{x},1/2$ [0,0,w] $\bar{x},x,1/2$ [0,0,w] $x,\bar{x},1/2$ [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>j</td>
<td>m.2'm' $x,x,0$ [0,0,w] $\bar{x},\bar{x},0$ [0,0,w] $\bar{x},x,0$ [0,0,w] $x,\bar{x},0$ [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>i</td>
<td>2'mm'. $0,1/2,z$ [u,0,0] $1/2,0,z$ [u,0,0] $0,1/2,\bar{z}$ [u,0,0] $1/2,0,\bar{z}$ [u,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>4'm'm' $1/2,1/2,z$ [0,0,w] $1/2,1/2,\bar{z}$ [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
<td>4'mm' $0,0,z$ [0,0,0] $0,0,\bar{z}$ [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>f</td>
<td>mmm'. $0,1/2,0$ [0,0,0] $1/2,0,0$ [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>mmm'. $0,1/2,1/2$ [0,0,0] $1/2,0,1/2$ [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>4/mm'm' $1/2,1/2,1/2$ [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>4/mm'm' $1/2,1/2,0$ [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4'/mmm' $0,0,1/2$ [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4'/mmm' $0,0,0$ [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] $p4mm1'$

- $a^* = a$
- $b^* = b$
- Origin at 0,0,z

Along [1,0,0] $p2mm1'$

- $a^* = b$
- $b^* = c$
- Origin at x,0,0

Along [1,1,0] $p_{21}$, 2m'm'

- $a^* = (-a + b)/2$
- $b^* = c$
- Origin at x-1/4, x+1/4, 0
Origin at center (4'/m'mm')

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)
(2) 2 0,0,z (2_z|0,0,0)
(3) 4' 0,0,z (4_z|0,0,0)
(4) 4' 0,0,z (4_z|0,0,0)
(5) 2' 0,y,0 (2_y|0,0,0)
(6) 2' x,0,0 (2_x|0,0,0)
(7) 2 0,y,0 (2_y|0,0,0)
(8) 2 0,y,0 (2_y|0,0,0)
(9) 1' 0,0,0 (1|0,0,0)
(10) m' x,y,0 (m_x|0,0,0)
(11) 4' 0,0,z; 0,0,0 (4_z|0,0,0)
(12) 4' 0,0,z; 0,0,0 (4_z|0,0,0)
(13) m x,0,z (m|0,0,0)
(14) m 0,y,z (m_y|0,0,0)
(15) m' x,y,z (m_x|0,0,0)
(16) m' x,y,z (m_x|0,0,0)
Continued

(1) \( t' (1,0,0) \)
(2) \( 2' 1/2,0,z \)
(3) \( 4' -1/2,1/2,z \)
(4) \( 4' 1/2,-1/2,z \)

For \((1,0,0)\)' + set

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Generators selected
(1); \( t'(1,0,0) \); \( t'(0,1,0) \); \( t(0,0,1) \); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

\( \begin{array}{cccc}
\text{Coordinates} & (0,0,0) + & (1,0,0)' + \\
\hline
(1) x,y,z [u,v,w] & (2) \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}] & (3) \bar{y}, \bar{x}, \bar{z} [\bar{v}, \bar{u}, \bar{w}] & (4) y, \bar{x}, z [\bar{v}, u, w] \\
(5) \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}] & (6) x, y, z [u, v, w] & (7) \bar{y}, x, \bar{z} [\bar{v}, u, w] & (8) y, x, \bar{z} [\bar{v}, u, w] \\
(9) x, \bar{y}, \bar{z} [u, v, w] & (10) \bar{x}, \bar{y}, z [\bar{u}, \bar{v}, \bar{w}] & (11) \bar{x}, \bar{y}, z [\bar{v}, \bar{u}, \bar{w}] & (12) y, \bar{x}, \bar{z} [\bar{v}, u, w] \\
(13) x, \bar{y}, \bar{z} [u, v, w] & (14) \bar{x}, \bar{y}, \bar{z} [\bar{u}, \bar{v}, \bar{w}] & (15) \bar{y}, x, \bar{z} [\bar{v}, u, w] & (16) y, x, z [v, u, w] \\
\end{array} \)

\( \begin{array}{cccc}
\text{Coordinates} & (0,0,0) + & (1,0,0)' + \\
\hline
x,1/2,z [u,0,w] & \bar{x},1/2,z [\bar{u},0,\bar{w}] & 1/2,x,z [0,0,w] & 1/2,\bar{x},z [0,0,\bar{w}] \\
\bar{x},1/2,\bar{z} [u,0,w] & x,1/2,\bar{z} [u,0,\bar{w}] & 1/2,x,\bar{z} [0,0,\bar{w}] & 1/2,\bar{x},\bar{z} [0,0,w] \\
x,0,z [0,0,v] & \bar{x},0,z [\bar{v},0,\bar{w}] & 0,x,z [v,0,0] & 0,\bar{x},z [v,0,\bar{w}] \\
\bar{x},0,\bar{z} [\bar{v},0,\bar{w}] & x,0,z [0,0,v] & 0,x,\bar{z} [v,0,0] & 0,\bar{x},\bar{z} [v,0,\bar{w}] \\
x,x,z [u,u,w] & \bar{x},x,\bar{z} [\bar{u},\bar{u},\bar{w}] & x,x,z [u,u,\bar{w}] & \bar{x},x,\bar{z} [u,u,\bar{w}] \\
\bar{x},x,\bar{z} [\bar{u},\bar{u},\bar{w}] & x,x,z [u,u,\bar{w}] & x,x,\bar{z} [u,u,\bar{w}] & \bar{x},x,\bar{z} [u,u,\bar{w}] \\
x,y,1/2 [u,v,0] & \bar{x},y,1/2 [\bar{u},\bar{v},0] & y,x,1/2 [v,u,0] & \bar{y},x,1/2 [\bar{v},u,0] \\
\bar{x},y,1/2 [\bar{u},\bar{v},0] & x,y,1/2 [u,v,0] & y,x,1/2 [v,u,0] & \bar{y},x,1/2 [\bar{v},u,0] \\
x,y,0 [u,v,0] & \bar{x},y,0 [\bar{u},\bar{v},0] & y,x,\bar{z} [v,0,0] & \bar{y},x,0 [\bar{v},0,0] \\
\bar{x},y,0 [\bar{u},\bar{v},0] & x,y,0 [u,v,0] & y,x,\bar{z} [v,0,0] & \bar{y},x,0 [\bar{v},0,0] \\
x,1/2,1/2 [u,0,0] & \bar{x},1/2,1/2 [\bar{u},0,\bar{w}] & 1/2,x,1/2 [0,0,\bar{w}] & 1/2,\bar{x},1/2 [0,0,w] \\
x,1/2,0 [u,0,0] & \bar{x},1/2,0 [\bar{u},0,\bar{w}] & 1/2,x,0 [0,0,\bar{w}] & 1/2,\bar{x},0 [0,0,w] \\
x,0,1/2 [0,v,0] & \bar{x},0,1/2 [\bar{v},0,\bar{w}] & 0,x,1/2 [v,0,0] & \bar{y},x,1/2 [\bar{v},0,0] \\
\end{array} \)
| 8 | l | m'2m' | x,0,0 [0,v,0] | x,0,0 [0,\(\bar{v},0\)] | 0,x,0 [v,0,0] | 0,\(\bar{x},0\) [\(\bar{v},0,0\)] |
| 8 | k | m'.2m' | x\(,x,1/2\) [u,u,0] | x\(,x,1/2\) [u,u,0] | x\(,x,1/2\) [u,u,0] | x\(,x,1/2\) [u,u,0] |
| 8 | j | m'.2m' | x\(,x,0\) [u,u,0] | x\(,x,0\) [u,u,0] | x\(,x,0\) [u,u,0] | x\(,x,0\) [u,u,0] |
| 8 | i | 2'mm' | 0,1/2,z [u,0,0] | 1/2,0,z [u,0,0] | 0,1/2,z [u,0,0] | 1/2,0,z [u,0,0] |
| 4 | h | 4m'm' | 1/2,1/2,z [0,0,w] | 1/2,1/2,z [0,0,w] | 0,1/2,z [0,0,w] | 0,1/2,z [0,0,w] |
| 4 | g | 4'mm' | 0,0,z [0,0,0] | 0,0,z [0,0,0] | 0,0,z [0,0,0] | 0,0,z [0,0,0] |
| 4 | f | m'm'm'. | 0,1/2,0 [u,0,0] | 1/2,0,0 [u,0,0] | 1/2,0,0 [u,0,0] | 1/2,0,0 [u,0,0] |
| 4 | e | m'm'm'. | 0,1/2,1/2 [u,0,0] | 1/2,0,1/2 [u,0,0] | 1/2,0,1/2 [u,0,0] | 1/2,0,1/2 [u,0,0] |
| 2 | d | 4/m'm'm' | 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |
| 2 | c | 4/m'm'm' | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 2 | b | 4'/m'm'm' | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |
| 2 | a | 4'/m'm'm' | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] \(p_p, 4m'm'\)

\[a^* = a\]

Along [1,0,0] \(p2mm1'\)

\[a^* = b\]

Origin at 1/2,1/2,z

\[b^* = b\]

Origin at x,0,0

\[a^* = (a+b)/2\]

Origin at x,x,0

\[b^* = c\]
**Origin** at center (4/mmm')

**Asymmetric unit**  
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y\]

### Symmetry Operations

For \((0,0,0)\) + set

1. \((1)|0,0,0\)
2. \((2)\ 0,0,z\)
3. \((3)\ 4^*\ 0,0,z\)
4. \((4)\ 4^*\ 0,0,0\)
5. \((5)\ 2'\ 0,y,0\)
6. \((6)\ 2'\ x,0,0\)
7. \((7)\ 2'\ x,x,0\)
8. \((8)\ 2'\ x,x,0\)
9. \((9)\ \bar{1}\ 0,0,0\)
10. \((10)\ m\ x,y,0\)
11. \((11)\ 4^*\ 0,0,z;\ 0,0,0\)
12. \((12)\ 4^*\ 0,0,0;\ 0,0,0\)
13. \((13)\ m'\ x,0,z\)
14. \((14)\ m'\ 0,y,z\)
15. \((15)\ m'\ x,x,z\)
16. \((16)\ m'\ x,x,z\)

For \((1,0,0)'\) + set

1. \((1)\ t'(1,0,0)\)
2. \((2)\ 2'\ 1/2,0,0\)
3. \((3)\ 4^*\ -1/2,1/2,0\)
4. \((4)\ 4^*\ 1/2,-1/2,0\)
5. \((5)\ 2\ 1/2,y,0\)
6. \((6)\ (2,1,0,0)\)
7. \((7)\ 2(1/2,1/2,0)\)
8. \((8)\ 2(1/2,-1,2,0)\)
9. \((9)\ \bar{1}\ 1/2,0,0\)
10. \((10)\ a(1,0,0)\)
11. \((11)\ 4^*\ -1/2,-1,2,0;\ 1/2,-1,2,0\)
12. \((12)\ 4^*\ 1/2,1,2,0;\ 1/2,1,2,0\)
13. \((13)\ a(1,0,0)\)
14. \((14)\ m\ 1/2,y,z\)
15. \((15)\ g(1/2,-1,2,0)\)
16. \((16)\ g(1/2,1,2,0)\)

**Generators selected**  
(1); \(t'(1,0,0); \ t'(0,1,0); \ t'(0,0,1); \ (2); \ (3); \ (5); \ (9).

### Positions

**Multiplicity, Wyckoff letter, Site Symmetry.**

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>32</td>
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<tr>
<td>16</td>
<td>t .m.</td>
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123.19.1017 - 2 - 2050
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Special Projections</th>
</tr>
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<tbody>
<tr>
<td>4' mm'</td>
<td>Along [0,0,1] p4mm1'</td>
</tr>
<tr>
<td>4 mm'</td>
<td>Along [1,0,0] p2mm1'</td>
</tr>
<tr>
<td>b* = b</td>
<td>Along [1,1,0] p$_{c'}$-2mm</td>
</tr>
<tr>
<td>a* = a</td>
<td>a* = b + a/2</td>
</tr>
<tr>
<td>Origin at 0,0,0</td>
<td>Origin at x,0,0</td>
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<tr>
<td></td>
<td>a* = (-a + b)/2</td>
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<tr>
<td></td>
<td>b* = c</td>
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<tr>
<td></td>
<td>Origin at x-1/4, x+1/4, 0</td>
</tr>
</tbody>
</table>

**Origin at 0,0,z**

### 16 s m'
- x,0,z [u,0,w] -> x,0,z [u,0,w]
- 0,x,z [0,u,w] -> 0,x,z [0,u,w]
- 0,x,z [0,u,w] -> 0,x,z [0,u,w]

### 16 r m'
- x,x,z [u,u,w] -> x,x,z [u,u,w]
- x,x,z [u,u,w] -> x,x,z [u,u,w]
- x,x,z [u,u,w] -> x,x,z [u,u,w]

### 16 q m'.
- x,y,1/2 [u,v,0] -> y,x,1/2 [v,u,0]
- x,y,1/2 [u,v,0] -> y,x,1/2 [v,u,0]
- x,y,1/2 [u,v,0] -> y,x,1/2 [v,u,0]

### 16 p m..
- x,y,0 [0,0,w] -> y,x,0 [0,0,w]
- y,x,0 [0,0,w] -> y,x,0 [0,0,w]
- y,x,0 [0,0,w] -> y,x,0 [0,0,w]

---

**Symmetry of Special Projections**

- **16 s m':** x,0,z [u,0,w] → x,0,z [u,0,w]
- **16 r m':** x,x,z [u,u,w] → x,x,z [u,u,w]
- **16 q m':** x,y,1/2 [u,v,0] → y,x,1/2 [v,u,0]
- **16 p m':** x,y,0 [0,0,w] → y,x,0 [0,0,w]

---

**Origin at 0,0,z**: 0,x,z [0,u,w] → 0,x,z [0,u,w]

---

**Origin at x,0,0**: x,x,z [u,u,w] → x,x,z [u,u,w]

---

**Origin at x-1/4, x+1/4, 0**: y,x,0 [0,0,w] → y,x,0 [0,0,w]
Origin at center (4/m) at 4/mcc

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(1) $0,0,0$

(2) $2,0,0,z$
(2) $(2z,0,0,0)$

(3) $4^+ 0,0,z$
(3) $(4z,0,0,0)$

(4) $4^- 0,0,z$
(4) $(4z^{-1},0,0,0)$

(5) 2
(5) $0,y,1/4$
(5) $(2,0,0,1/2)$

(6) $2,x,0,1/4$
(6) $(2z,0,0,1/2)$

(7) $2,x,x,1/4$
(7) $(2y,0,0,1/2)$

(8) $2,x,x,1/4$
(8) $(2y,0,0,1/2)$

(9) $\overline{1}$
(9) $0,0,0$
(9) $(1,0,0,0)$

(10) $m,x,y,0$
(10) $(m,0,0,0)$

(11) $\overline{4}^+ 0,0,z; 0,0,0$
(11) $\overline{4}z,0,0,0$

(12) $\overline{4}^- 0,0,z; 0,0,0$
(12) $\overline{4}z^{-1},0,0,0$

(13) $c(0,0,1/2) x,0,z$
(13) $(m,0,0,1/2)$

(14) $c(0,0,1/2) 0,y,z$
(14) $(m,0,0,1/2)$

(15) $c(0,0,1/2) x,x,z$
(15) $(m,0,0,1/2)$

(16) $c(0,0,1/2) x,x,z$
(16) $(m,0,0,1/2)$
**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>16 n 1</td>
<td>n</td>
<td>1 (1) x,y,z [u,v,w] (2) x, y, z [u,v,w] (3) y, x, z [v,u,w] (4) y, x, z [v,u,w] (5) x, y, z +1/2 [u,v,w] (6) x, y, z +1/2 [u,v,w] (7) y, x, z +1/2 [v,u,w] (8) y, x, z +1/2 [v,u,w] (9) x, y, z [u,v,w] (10) x,y,z [u,v,w] (11) y,x,z [v,u,w] (12) y,x,z [v,u,w] (13) x,y,z+1/2 [u,v,w] (14) x,y,z+1/2 [v,u,w] (15) y,x,z+1/2 [v,u,w] (16) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8 m m..</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w] y,x,0 [0,0,w] y,x,0 [0,0,w]</td>
</tr>
<tr>
<td>8 l .2</td>
<td>x,1/2,1/4 [u,v,0]</td>
<td>1/2,x,1/4 [0,0,u] 1/2,x,1/4 [0,0,u]</td>
</tr>
<tr>
<td>8 k .2</td>
<td>x,0,1/4 [u,0,v]</td>
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<td>0,0,3/4 [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1]  p4mm1'
\(a^* = a\)  \(b^* = b\)
Origin at 0,0,z

Along [1,0,0]  p_{2a'2m'm'}
\(a^* = -c/2\)  \(b^* = b\)
Origin at x,0,1/4

Along [1,1,0]  p_{2a'2m'm'}
\(a^* = -c/2\)  \(b^* = (-a + b)/2\)
Origin at x,x,1/4
**P4/mcc1' P4/m2/c2/c1'**

**Tetragonal**

**Origin** at center (4/m1') at 4/mcc1'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

For 1 + set

1. \(1\) 1
   
   \[
   (1|0,0,0) \\
   (1|0,0,0)
   \]

2. \(2\) \(0,0,z\)
   
   \[
   (2_z|0,0,0) \\
   (2_z|0,0,0)
   \]

3. \(4^+\) \(0,0,z\)
   
   \[
   (4_z|0,0,0) \\
   (4_z^{-1}|0,0,0)
   \]

4. \(4^-\) \(0,0,z\)
   
   \[
   (4_z^{-1}|0,0,0) \\
   (4_z^{-1}|0,0,0)
   \]

5. \(2\) \(0,y,1/4\)
   
   \[
   (2_y|0,0,1/2) \\
   (2_y|0,0,1/2)
   \]

6. \(2\) \(x,0,1/4\)
   
   \[
   (2_x|0,0,1/2) \\
   (2_x|0,0,1/2)
   \]

7. \(2\) \(x,x,1/4\)
   
   \[
   (2_{xx}|0,0,1/2) \\
   (2_{xx}|0,0,1/2)
   \]

8. \(2\) \(x,x,1/4\)
   
   \[
   (2_{xx}|0,0,1/2) \\
   (2_{xx}|0,0,1/2)
   \]

9. \(\bar{1}\) \(0,0,0\)
   
   \[
   (1|0,0,0) \\
   (1|0,0,0)
   \]

10. \(m\) \(x,y,0\)
    
    \[
    (m_y|0,0,0) \\
    (m_y|0,0,0)
    \]

11. \(\bar{4}^+\) \(0,0,z; 0,0,0\)
    
    \[
    (\bar{4}_z|0,0,0) \\
    (\bar{4}_z^{-1}|0,0,0)
    \]

12. \(\bar{4}^-\) \(0,0,z; 0,0,0\)
    
    \[
    (\bar{4}_z^{-1}|0,0,0) \\
    (\bar{4}_z^{-1}|0,0,0)
    \]

13. \(c\) \((0,0,1/2)\) \(x,0,z\)
    
    \[
    (c_{|y}|0,0,1/2) \\
    (m_{xy}|0,0,1/2)
    \]

14. \(c\) \((0,0,1/2)\) \(0,y,z\)
    
    \[
    (m_{xy}|0,0,1/2) \\
    (m_{xy}|0,0,1/2)
    \]

15. \(c\) \((0,0,1/2)\) \(x,x,z\)
    
    \[
    (m_{xy}|0,0,1/2) \\
    (m_{xy}|0,0,1/2)
    \]

16. \(c\) \((0,0,1/2)\) \(x,x,z\)
    
    \[
    (m_{xy}|0,0,1/2) \\
    (m_{xy}|0,0,1/2)
    \]
For $1^+ +$ set

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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Generators selected  (1); (1,0,0); (0,1,0); (0,0,1); (2); (3); (5); (9); 1'.
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<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>2</td>
<td>c</td>
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<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
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<tr>
<td>2</td>
<td>b</td>
<td>4/m..1'</td>
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<tr>
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<td>a</td>
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<td>0,0,3/4 [0,0,0]</td>
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</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'

\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)

Origin at 0,0,z

Along [1,0,0] p2mm1'

\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}/2 \)

Origin at x,0,0

Along [1,1,0] p2mm1'

\( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)

Origin at x,x,0
Origin at center (4/m') at 4/m'cc

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
    (1 | 0,0,0)

(5) 2' 0,y,1/4
    (2|0,0,1/2)'

(9) T' 0,0,0
    (1 | 0,0,0)'

(13) c (0,0,1/2) x,0,z
     (m|0,0,1/2)

(2) 2 0,0,z
    (2|0,0,0)

(6) 2' x,0,1/4
    (2|0,0,1/2)'

(10) m' x,y,0
     (m|0,0,0)'

(14) c (0,0,1/2) 0,y,z
     (m|0,0,1/2)

(3) 4+ 0,0,z
    (4|0,0,0)

(7) 2' x,x,1/4
    (2|0,0,1/2)'

(11) 4++ 0,0,z; 0,0,0
     (4|0,0,0)'

(12) 4++ 0,0,z; 0,0,0
     (4|0,0,1/2)'

(4) 4' 0,0,z
    (4|0,0,0)

(8) 2' x,x,1/4
    (2|0,0,1/2)'

(15) c (0,0,1/2) x,x,z
     (m|0,0,1/2)

(16) c (0,0,1/2) x,x,z
     (m|0,0,1/2)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>2</td>
<td>b</td>
<td>4/m'..</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>42'2'</td>
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</table>

Continued 124.3.1020 P4/m'cc
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Basis Vectors</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p4mm</td>
<td>$a^* = a$</td>
<td>0,0,z</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b$</td>
<td></td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>$p_{2a'}2m'm'$</td>
<td>$a^* = -c/2$</td>
<td>x,0,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b$</td>
<td></td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>$p_{2a'}2m'm'$</td>
<td>$a^* = -c/2$</td>
<td>x,x,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = (-a + b)/2$</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (4'/m) at 4'/mc'c

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

1. 1 (1 | 0,0,0)
2. 2 0,0,z (2z | 0,0,0)
3. 4' 0,0,z (4z | 0,0,0)
4. 4' 0,0,z (4z | 0,0,0)
5. 2' 0,y,1/4 (2y | 0,0,1/2)
6. 2' x,0,1/4 (2x | 0,0,1/2)
7. 2 x,x,1/4 (2x | 0,0,1/2)
8. 2 x,x,1/4 (2x | 0,0,1/2)
9. 1 0,0,0 (1 | 0,0,0)
10. m x,y,0 (mz | 0,0,0)
11. 4+m 0,0,z; 0,0,0 (4z | 0,0,0)
12. 4+m 0,0,z; 0,0,0 (4z | 0,0,0)
13. c' (0,0,1/2) x,0,z (mz | 0,0,1/2)
14. c' (0,0,1/2) 0,y,z (mz | 0,0,1/2)
15. c (0,0,1/2) x,x,z (mz | 0,0,1/2)
16. c (0,0,1/2) x,x,z (mz | 0,0,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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</tr>
<tr>
<td>16</td>
<td>n</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z +1/2 [u, v, w] (6) x, y, z +1/2 [u, v, w] (7) y, x, z +1/2 [v, u, w] (8) y, x, z +1/2 [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(9) x, y, z [u, v, w] (10) x, y, z [u, v, w] (11) y, x, z [v, u, w] (12) y, x, z [v, u, w]</td>
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<tr>
<td></td>
<td>(13) x, y, z +1/2 [u, v, w] (14) x, y, z +1/2 [u, v, w] (15) y, x, z +1/2 [v, u, w] (16) y, x, z +1/2 [v, u, w]</td>
</tr>
<tr>
<td>8</td>
<td>m</td>
</tr>
<tr>
<td></td>
<td>(15) x, y, 1/2 [0,0,w] x,y,1/2 [0,0,w] y,x,1/2 [0,0,w] y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>l</td>
</tr>
<tr>
<td></td>
<td>(15) x, 1/2,3/4 [0,v,w] x,1/2,3/4 [0,v,w] 1/2,x,3/4 [v,0,w] 1/2,x,3/4 [v,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>k</td>
</tr>
<tr>
<td></td>
<td>(15) x, 0,3/4 [0,v,w] x,0,3/4 [0,v,w] 0,x,3/4 [v,0,w] 0,x,3/4 [v,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>j</td>
</tr>
<tr>
<td></td>
<td>(15) x, x, 3/4 [u,u,0] x,x,3/4 [u,u,0] x,x,3/4 [u,u,0] x,x,3/4 [u,u,0]</td>
</tr>
<tr>
<td>8</td>
<td>i</td>
</tr>
<tr>
<td></td>
<td>(15) 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z +1/2 [0,0,w] 0,1/2,z +1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
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<tr>
<td></td>
<td>(15) 0,0,z [0,0,0] 0,0,z [0,0,0] 0,0,z [0,0,0] 0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>f</td>
</tr>
<tr>
<td></td>
<td>(15) 0,1/2,0 [0,0,w] 0,1/2,0 [0,0,w] 0,1/2,1/2 [0,0,w] 0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
</tr>
<tr>
<td></td>
<td>(15) 1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2</td>
<td>c</td>
</tr>
<tr>
<td></td>
<td>(15) 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
</tr>
</tbody>
</table>

124.4.1021 - 2 - 2062
Symmetry of Special Projections

Along [0,0,1]  p4mm1'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0]  p 2'mm'  
\( \mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at x,0,0

Along [1,1,0]  p_{2a'} 2m'm'  
\( \mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)  
Origin at x,x,1/4
P4'/mcc'  
124.5.1022

4'/mmm'  
P4'/m2/c2'/c'

Tetragonal

**Origin** at center (4'/m) at 4'/mcc'

**Asymmetric unit**  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

**Symmetry Operations**

1. $1$
   
2. $2 \ x,0,0$  
   \( (2_x,0,0) \)

3. $4^{+} \ x,0,0$  
   \( (4_x,0,0,0') \)

4. $4^{-} \ x,0,0$  
   \( (4^{-}_x,0,0,0') \)

5. $2 \ y,1/4$  
   \( (2_y,0,0,1/2) \)

6. $2' \ x,0,1/4$  
   \( (2_x,0,0,1/2) \)

7. $2' \ x,0,1/4$  
   \( (2_x,0,0,1/2) \)

8. $2' \ x,0,1/4$  
   \( (2_x,0,0,1/2) \)

9. $\bar{1} \ 0,0,0$  
   \( (1,0,0,0) \)

10. $m \ x,y,0$  
    \( (m_x,0,0,0) \)

11. $4^{+} \ x,0,0,0$  
    \( (4^{+}_x,0,0,0') \)

12. $4^{-} \ x,0,0,0$  
    \( (4^{-}_x,0,0,0') \)

13. $c \ (0,0,1/2) \ x,0,z$  
    \( (m,0,0,1/2) \)

14. $c \ (0,0,1/2) \ 0,y,z$  
    \( (m,0,0,1/2) \)

15. $c' \ (0,0,1/2) \ x,x,z$  
    \( (m_x,0,0,1/2) \)

16. $c' \ (0,0,1/2) \ x,x,z$  
    \( (m_x,0,0,1/2) \)

124.5.1022 - 1 - 2064
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 n 1</td>
<td>(1) x, y, z [u, v, w]</td>
<td>(2) x, y, z [u, v, w]</td>
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<td>(3) y, x, z [v, u, w]</td>
<td>(4) y, x, z [v, u, w]</td>
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<tr>
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<td>(5) x, y, z+1/2 [u, v, w]</td>
<td>(6) x, y, z+1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(7) y, x, z+1/2 [v, u, w]</td>
<td>(8) y, x, z+1/2 [v, u, w]</td>
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<td></td>
<td>(9) x, y, z [u, v, w]</td>
<td>(10) x, y, z [u, v, w]</td>
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<tr>
<td></td>
<td>(11) y, x, z [v, u, w]</td>
<td>(12) y, x, z [v, u, w]</td>
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<td>(13) x, y, z+1/2 [u, v, w]</td>
<td>(14) x, y, z+1/2 [u, v, w]</td>
</tr>
<tr>
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<td>(16) y, x, z+1/2 [v, u, w]</td>
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<tr>
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<td>x, y, 0 [0, 0, w]</td>
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<td>y, x, 0 [0, 0, w]</td>
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<td>y, x, 1/2 [0, 0, w]</td>
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<td>8 l .2</td>
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<td>x, 1/2, 1/4 [u, 0, 0]</td>
<td>1/2, x, 1/4 [0, u, 0]</td>
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<td>1/2, x, 1/4 [0, u, 0]</td>
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<td>1/2, x, 3/4 [0, u, 0]</td>
<td>1/2, x, 3/4 [0, u, 0]</td>
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<td>8 k .2</td>
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<td>x, 0, 1/4 [0, u, 0]</td>
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<td>x, 0, 1/4 [0, u, 0]</td>
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<td>0, x, 1/4 [0, u, 0]</td>
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<tr>
<td>8 j .2'</td>
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<td>x, x, 1/4 [u, u, w]</td>
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<td>x, x, 1/4 [u, u, w]</td>
<td>x, x, 1/4 [u, u, w]</td>
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<tr>
<td></td>
<td>x, x, 3/4 [u, u, w]</td>
<td>x, x, 3/4 [u, u, w]</td>
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<td>x, x, 3/4 [u, u, w]</td>
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<td>1/2, 0, z [0, 0, w]</td>
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<td>1/2, 0, z+1/2 [0, 0, w]</td>
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<td>4 f 222.</td>
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<td>0, 1/2, 1/2 [0, 0, w]</td>
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<td>2 d 4'/m..</td>
<td>1/2, 1/2, 0 [0, 0, 0]</td>
<td>1/2, 1/2, 1/2 [0, 0, 0]</td>
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<tr>
<td>2 c 4'/22'</td>
<td>1/2, 1/2, 1/4 [0, 0, 0]</td>
<td>1/2, 1/2, 3/4 [0, 0, 0]</td>
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<tr>
<td>2 b 4'/m..</td>
<td>0, 0, 0 [0, 0, 0]</td>
<td>0, 0, 1/2 [0, 0, 0]</td>
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<tr>
<td>2 a 4'/22'</td>
<td>0, 0, 1/4 [0, 0, 0]</td>
<td>0, 0, 3/4 [0, 0, 0]</td>
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</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>a* =</th>
<th>b* =</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p4mm1'</td>
<td>a</td>
<td>b</td>
<td>0,0,z</td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p2a'-2m'm'</td>
<td>-c/2</td>
<td>b</td>
<td>x,0,1/4</td>
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<tr>
<td>[1,1,0]</td>
<td>p2'mm'</td>
<td>-c/2</td>
<td>-(a+b)/2</td>
<td>x,x,0</td>
</tr>
</tbody>
</table>

- a* = a, b* = b
- a* = -c/2, b* = b
- a* = -c/2, b* = -(a+b)/2
Origin at center (4'/m') at 4'/m'c'c

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2  0,0,z  
(2|0,0,0)

(3) 4'  0,0,z  
(4|0,0,0)

(4) 4' - 0,0,z  
(4|-0,0,0)

(5) 2  0,y,1/4  
(2|0,0,1/2)

(6) 2  x,0,1/4  
(2|0,0,1/2)

(7) 2'  x,x,1/4  
(2|x,0,1/2)

(8) 2'  x,x,1/4  
(2|x,0,1/2)

(9) 1'  0,0,0  
(1|0,0,0)

(10) m'  x,y,0  
(m|0,0,0)

(11) 4'  0,0,z; 0,0,0  
(4|0,0,0)

(12) 4'  0,0,z; 0,0,0  
(4|-0,0,0)

(13) c' (0,0,1/2)  x,0,z  
(m|0,0,1/2)

(14) c' (0,0,1/2)  0,y,z  
(m|0,0,1/2)

(15) c (0,0,1/2)  x,x,z  
(m|x,0,1/2)

(16) c (0,0,1/2)  x,x,z  
(m|x,0,1/2)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
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<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>(8) y,x,z+1/2 [v,u,w]</td>
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<td>(9) x,y,z [u,v,w]</td>
<td>(10) x,y,z+1/2 [u,v,w]</td>
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<td></td>
<td>(11) y,x,z [v,u,w]</td>
<td>(12) y,x,z [v,u,w]</td>
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<td>(13) x,y,z+1/2 [u,v,w]</td>
<td>(14) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(15) y,x,z+1/2 [v,u,w]</td>
<td>(16) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8 m m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [u,v,0]</td>
<td>y,x,1/2 [v,u,0]</td>
</tr>
<tr>
<td>8 l .2</td>
<td>x,1/2,1/4 [u,0,0]</td>
<td>1/2,x,1/4 [0,u,0]</td>
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<tr>
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<td>x,1/2,3/4 [u,0,0]</td>
<td>1/2,x,3/4 [0,u,0]</td>
</tr>
<tr>
<td>8 k .2</td>
<td>x,0,1/4 [u,0,0]</td>
<td>0,x,1/4 [0,u,0]</td>
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<td>x,0,3/4 [u,0,0]</td>
<td>0,x,3/4 [0,u,0]</td>
</tr>
<tr>
<td>8 j .2'</td>
<td>x,x,1/4 [u,u,w]</td>
<td>x,x,1/4 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,3/4 [u,u,w]</td>
<td>x,x,3/4 [u,u,w]</td>
</tr>
<tr>
<td>8 i 2'</td>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 h 4'..</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 g 4'..</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 f 222.</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 e 2/m'..</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 d 4'm'..</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 4'22'</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 b 4'm'..</td>
<td>0,0,0 [0,0,0]</td>
<td>0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 a 4'22'</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1]  p4'm'm  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0]  p 2m'm'  
\( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at x,0,0

Along [1,1,0]  p 2a* 2m'm'  
\( \mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)  
Origin at x,x,0
Origin at center (4/m) at 4/mc'c'

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

1. 1
   (1|0,0,0)

2. 2 0,0,z
   (2z|0,0,0)

3. 4+ 0,0,z
   (4z|0,0,0)

4. 4− 0,0,z
   (4z⁻¹|0,0,0)

5. 2' 0,y,1/4
   (2y|0,0,1/2')

6. 2' x,0,1/4
   (2x|0,0,1/2')

7. 2' x,x,1/4
   (2xy|0,0,1/2')

8. 2' x,x,1/4
   (2xy|0,0,1/2')

9. 1 0,0,0
   (1|0,0,0)

10. m x,y,0
    (m|0,0,0)

11. 4+ 0,0,z; 0,0,0
    (4z|0,0,0)

12. 4− 0,0,z; 0,0,0
    (4z⁻¹|0,0,0)

13. c' (0,0,1/2) x,0,z
    (m|0,0,1/2')

14. c' (0,0,1/2) 0,y,z
    (m|0,0,1/2')

15. c' (0,0,1/2) x,x,z
    (m|0,0,1/2')

16. c' (0,0,1/2) x,x,z
    (m|0,0,1/2')
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>n</td>
</tr>
<tr>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
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<tr>
<td></td>
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<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| 8            | m           |
| 1            | .2'         |
|              | x,1/2,1/4 [0,v,w] | x,1/2,1/4 [0,v,w] | 1/2,x,1/4 [v,0,w] | 1/2,x,1/4 [v,0,w] |
|              | .2'         |
| 8            | k           |
| 1            | .2'         |
|              | x,0,1/4 [0,v,w] | x,0,1/4 [0,v,w] | 0,x,1/4 [v,0,w] | 0,x,1/4 [v,0,w] |
|              | .2'         |
| 8            | j           |
| 1            | .2'         |
|              | x,x,1/4 [u,u,w] | x,x,1/4 [u,u,w] | x,x,1/4 [u,u,w] | x,x,1/4 [u,u,w] |
|              | .2'         |
| 8            | i           |
| 1            | .2'         |
|              | 0,1/2,z [0,0,w] | 1/2,0,z [0,0,w] | 0,1/2,z+1/2 [0,0,w] | 1/2,0,z+1/2 [0,0,w] |
|              | .2'         |
| 4            | h           |
| 1            | .2'         |
|              | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] |
|              | .2'         |
| 4            | f           |
| 1            | .2'         |
|              | 0,1/2,1/4 [0,0,w] | 1/2,0,1/4 [0,0,w] | 1/2,0,1/4 [0,0,w] | 1/2,0,1/4 [0,0,w] |
|              | .2'         |
| 4            | e           |
| 1            | .2'         |
|              | 0,1/2,0 [0,0,w] | 1/2,0,0 [0,0,w] | 0,1/2,1/2 [0,0,w] | 1/2,0,1/2 [0,0,w] |
|              | .2'         |
| 2            | d           |
| 1            | .2'         |
|              | 1/2,1/2,0 [0,0,w] | 1/2,1/2,1/2 [0,0,w] | 1/2,1/2,1/2 [0,0,w] | 1/2,1/2,1/2 [0,0,w] |
|              | .2'         |
| 2            | c           |
| 1            | .2'         |
|              | 1/2,1/2,1/4 [0,0,w] | 1/2,1/2,3/4 [0,0,w] | 1/2,1/2,3/4 [0,0,w] | 1/2,1/2,3/4 [0,0,w] |
|              | .2'         |
| 2            | b           |
| 1            | .2'         |
|              | 0,0,0 [0,0,w] | 0,0,1/2 [0,0,w] | 0,0,1/2 [0,0,w] | 0,0,1/2 [0,0,w] |
|              | .2'         |
| 2            | a           |
| 1            | .2'         |
|              | 0,0,1/4 [0,0,w] | 0,0,3/4 [0,0,w] | 0,0,3/4 [0,0,w] | 0,0,3/4 [0,0,w] |
## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Transformation</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4mm'</td>
<td>$a^* = a$</td>
<td>0,0,z</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b$</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p 2'mm'</td>
<td>$a^* = -c/2$</td>
<td>x,0,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b$</td>
<td></td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p 2'mm'</td>
<td>$a^* = -c/2$</td>
<td>x,x,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = (-a + b)/2$</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (4'/m') at 4'/m'cc'

Asymmetric unit
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\]

Symmetry Operations

1. \(1\) 1
2. \(2\) 0,0,z
3. \(4^+\) 0,0,z
4. \(4^-\) 0,0,z
5. \(2'\) 0,y,1/4
6. \(2^*\) x,0,1/4
7. \(2\) x,x,1/4
8. \(2\) x,x,1/4
9. \(\bar{1}\) 0,0,0
10. \(m'\) x,y,0
11. \(\bar{4}^+\) 0,0,z; 0,0,0
12. \(\bar{4}^-\) 0,0,z; 0,0,0
13. \(c(0,0,1/2)\) x,0,z
14. \(c(0,0,1/2)\) 0,y,z
15. \(c'(0,0,1/2)\) x,x,z
16. \(c'(0,0,1/2)\) x,x,z

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Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>16 n 1</td>
<td>(1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(5) x, y, z +1/2 [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(9) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(13) x, y, z +1/2 [u, v, w]</td>
</tr>
<tr>
<td>8 m m'..</td>
<td>x, y, 0 [u, v, 0]</td>
</tr>
<tr>
<td></td>
<td>x, y, 1/2 [u, v, 0]</td>
</tr>
<tr>
<td>8 l .2'</td>
<td>x, 1/2, 1/4 [0, v, w]</td>
</tr>
<tr>
<td></td>
<td>x, 1/2, 3/4 [0, v, w]</td>
</tr>
<tr>
<td>8 k .2'</td>
<td>x, 0, 1/4 [0, v, w]</td>
</tr>
<tr>
<td></td>
<td>x, 0, 3/4 [0, v, w]</td>
</tr>
<tr>
<td>8 j .2</td>
<td>x, x, 1/4 [u, u, 0]</td>
</tr>
<tr>
<td></td>
<td>x, x, 3/4 [u, u, 0]</td>
</tr>
<tr>
<td>8 i 2..</td>
<td>0, 1/2, z [0, 0, w]</td>
</tr>
<tr>
<td></td>
<td>0, 1/2, z [0, 0, w]</td>
</tr>
<tr>
<td>4 h 4'..</td>
<td>1/2, 1/2, z [0, 0, 0]</td>
</tr>
<tr>
<td>4 g 4'..</td>
<td>0, 0, z [0, 0, 0]</td>
</tr>
<tr>
<td>4 f 22'2'</td>
<td>0, 1/2, 1/4 [0, 0, w]</td>
</tr>
<tr>
<td>4 e 2/m'..</td>
<td>0, 1/2, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>2 d 4/m'..</td>
<td>1/2, 1/2, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>2 c 4'22</td>
<td>1/2, 1/2, 1/4 [0, 0, 0]</td>
</tr>
<tr>
<td>2 b 4'm'..</td>
<td>0, 0, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>2 a 4'22</td>
<td>0, 0, 1/4 [0, 0, 0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p4'mm'
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p_2a'-2m'm'
\[ a^* = -c/2 \quad b^* = b \]
Origin at x,0,0

Along [1,1,0] p 2m'm'
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
**Origin** at center (4/m') at 4/m'c'c'

**Asymmetric unit**

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}\]

**Symmetry Operations**

1. \(1\)
   - \((1|0,0,0)\)

2. \(2\)
   - \((0,0,z)\)
   - \((2_z|0,0,0)\)

3. \(4^+\)
   - \((0,0,z)\)
   - \((4_z|0,0,0)\)

4. \(4^-\)
   - \((0,0,z)\)
   - \((4_z^{-1}|0,0,0)\)

5. \(2\)
   - \((0,y,1/4)\)
   - \((2_y|0,0,1/2)\)

6. \(2\)
   - \((x,0,1/4)\)
   - \((2_z|0,0,1/2)\)

7. \(2\)
   - \((x,x,1/4)\)
   - \((2_{xy}|0,0,1/2)\)

8. \(2\)
   - \((x,x,1/4)\)
   - \((2_{xy}|0,0,1/2)\)

9. \(\overline{1}\)
   - \((0,0,0)\)
   - \((1|0,0,0)\)'s

10. \(m'\)
    - \((m_x|0,0,0)\)'
    - \((m_y|0,0,1/2)\)'

11. \(4^+\)·
    - \((0,0,z)\)
    - \((4_z|0,0,0)\)'

12. \(4^-\)·
    - \((0,0,z)\)
    - \((4_z^{-1}|0,0,0)\)'

13. \(c'\)·
    - \((0,0,1/2)\)
    - \((m_x|0,0,1/2)\)'

14. \(c'\)·
    - \((0,0,1/2)\)
    - \((m_y|0,0,1/2)\)'

15. \(c'\)·
    - \((0,0,1/2)\)
    - \((m_{xy}|0,0,1/2)\)'

16. \(c'\)·
    - \((0,0,1/2)\)
    - \((m_{xy}|0,0,1/2)\)'

**Remarks**

- **Origin at center (4/m') at 4/m'c'c'**
- **Asymmetric unit**
  - \(0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq \frac{1}{4}\)
- **Symmetry Operations**
  - (1) \(1\)
  - (2) \(2\)
  - (3) \(4^+\)
  - (4) \(4^-\)
  - (5) \(2\)
  - (6) \(2\)
  - (7) \(2\)
  - (8) \(2\)
  - (9) \(\overline{1}\)
  - (10) \(m'\)
  - (11) \(4^+\)·
  - (12) \(4^-\)·
  - (13) \(c'\)
  - (14) \(c'\)
  - (15) \(c'\)
  - (16) \(c'\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>n</td>
<td>1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>m</td>
<td>m'.. x,y,0 [u,v,0] (5) x,y,z+1/2 [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) y,x,z+1/2 [v,u,w] (8) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>l</td>
<td>.2. x,1/2,1/4 [u,0,0] (9) x,y,z [u,v,w] (10) x,y,z [u,v,w] (11) y,x,z [v,u,w] (12) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>k</td>
<td>.2. x,0,1/4 [u,0,0] (13) x,y,z+1/2 [u,v,w] (14) x,y,z+1/2 [u,v,w] (15) y,x,z+1/2 [v,u,w] (16) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>j</td>
<td>.2. x,x,1/4 [u,u,0] (17) x,x,1/4 [u,u,0] (18) x,x,1/4 [u,u,0] (19) x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td>8</td>
<td>i</td>
<td>2.. 0,1/2,z [0,0,w] (20) 0,1/2,z [0,0,w] (21) 0,1/2,z [0,0,w] (22) 0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>4.. 1/2,1/2,z [0,0,w] (23) 1/2,1/2,z [0,0,w] (24) 1/2,1/2,z [0,0,w] (25) 1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
<td>4.. 0,0,z [0,0,w] (26) 0,0,z [0,0,w] (27) 0,0,z [0,0,w] (28) 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>f</td>
<td>222. 1/2,1/4 [0,0,0] (29) 1/2,1/4 [0,0,0] (30) 1/2,1/4 [0,0,0] (31) 1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>2/m'.. 0,1/2,0 [0,0,0] (32) 0,1/2,0 [0,0,0] (33) 0,1/2,0 [0,0,0] (34) 0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>4/m'.. 1/2,1/2,0 [0,0,0] (35) 1/2,1/2,0 [0,0,0] (36) 1/2,1/2,0 [0,0,0] (37) 1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>422 1/2,1/2,1/4 [0,0,0] (38) 1/2,1/2,1/4 [0,0,0] (39) 1/2,1/2,1/4 [0,0,0] (40) 1/2,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4/m'.. 0,0,0 [0,0,0] (41) 0,0,0 [0,0,0] (42) 0,0,0 [0,0,0] (43) 0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>422 0,0,1/4 [0,0,0] (44) 0,0,1/4 [0,0,0] (45) 0,0,1/4 [0,0,0] (46) 0,0,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p4m'm'
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p 2m'm'
\[ a^* = b \quad b^* = c/2 \]
Origin at x,0,0

Along [1,1,0] p 2m'm'
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
Origin at center (4/m) at 4/mcc

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\)

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 4^+ \quad 0,0,z \\
(4) & \quad 4^- \quad 0,0,z \\
(5) & \quad 2 \quad 0,y,1/4 \\
(6) & \quad 2 \quad x,0,1/4 \\
(7) & \quad 2 \quad x,x,1/4 \\
(8) & \quad 2 \quad x,x,1/4 \\
(9) & \quad \overline{1} \quad 0,0,0 \\
(10) & \quad m \quad x,y,0 \\
(11) & \quad 4^+ \quad 0,0,z; \quad 0,0,0 \\
(12) & \quad 4^- \quad 0,0,z; \quad 0,0,0 \\
(13) & \quad c \quad (0,0,1/2) \quad x,0,z \\
(14) & \quad c \quad (0,0,1/2) \quad 0,y,z \\
(15) & \quad c \quad (0,0,1/2) \quad x,x,z \\
(16) & \quad c \quad (0,0,1/2) \quad x,x,z
\end{align*}
\]
For $(1,0,0)' + \text{set}$

(1) $t'(1,0,0)$
(1,0,0)'

(2) $2'(1/2,0,z)$
(1,0,0)'

(3) $4^{+}\cdot -1/2,1/2,z$
(1,0,0)'

(4) $4^{+}\cdot 1/2,-1/2,z$
(1,0,0)'

(5) $2'1/2,y,1/4$
(2,1,0,1/2)'

(6) $2'(1,0,0)x,0,1/4$
(2,1,0,1/2)'

(7) $2'(1/2,1/2,0)x+1/2,x,1/4$
(2,1,0,1/2)'

(8) $2'(1/2,-1/2,0)x+1/2,\overline{x},1/4$
(2,1,0,1/2)'

(9) $1/2,0,z$
(1,0,0)'

(10) $4^{+}\cdot 1/2,-1/2,z; 1/2,-1/2,0$
(1,0,0)'

(11) $4^{+}\cdot 1/2,1/2,z; 1/2,1/2,0$
(1,0,0)'

(12) $2^{+}\cdot 1,0,1/2$
(2,1,0,1/2)'

(13) $c'(0,0,1/2)1/2,y,z$
(1,0,0)'

(14) $n'(1/2,1/2,1/2)x+1/2,x,z$
(1,0,0)'

(15) $n'(1/2,1/2,1/2)x+1/2,x,z$
(1,0,0)'

(16) $n'(1/2,1/2,1/2)x+1/2,x,z$
(1,0,0)'

Generators selected (1); $t'(1,0,0)$; $t'(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>32</td>
<td>n</td>
</tr>
<tr>
<td>$1$</td>
<td>$x,y,z$ [u,v,w]</td>
</tr>
<tr>
<td>16</td>
<td>m</td>
</tr>
<tr>
<td>$x,y,0$ [0,0,w]</td>
<td>$\bar{x},\bar{y},0$ [\overline{0},0,\overline{w}]</td>
</tr>
<tr>
<td>16</td>
<td>l</td>
</tr>
<tr>
<td>$x,1/2,1/4$ [0,v,w]</td>
<td>$\bar{x},1/2,1/4$ [\overline{0},v,w]</td>
</tr>
<tr>
<td>16</td>
<td>k</td>
</tr>
<tr>
<td>$x,0,1/4$ [u,0,0]</td>
<td>$\bar{x},0,1/4$ [\overline{u},0,0]</td>
</tr>
<tr>
<td>16</td>
<td>j</td>
</tr>
<tr>
<td>$x,x,1/4$ [u,u,0]</td>
<td>$\bar{x},x,1/4$ [\overline{u},u,0]</td>
</tr>
<tr>
<td>16</td>
<td>i</td>
</tr>
<tr>
<td>$x,x,3/4$ [u,u,0]</td>
<td>$\bar{x},x,3/4$ [\overline{u},u,0]</td>
</tr>
<tr>
<td>16</td>
<td>h</td>
</tr>
<tr>
<td>$0,1/2,z$ [u,v,0]</td>
<td>$1/2,0,z$ [\overline{v},\overline{u},0]</td>
</tr>
<tr>
<td>8</td>
<td>4'</td>
</tr>
<tr>
<td>$1/2,1/2,z$ [0,0,0]</td>
<td>$1/2,1/2,\bar{z}+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
</tr>
<tr>
<td>$0,0,z$ [0,0,w]</td>
<td>$0,0,\bar{z}+1/2$ [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
</tr>
<tr>
<td>$0,1/2,1/4$ [v,0,0]</td>
<td>$1/2,0,1/4$ [v,0,0]</td>
</tr>
</tbody>
</table>
Continued

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P₃ 4/mcc

8  e  2'/m..  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]
4  d  4'/m..  1/2,1/2,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]
4  c  4'2'2  1/2,1/2,1/4 [0,0,0]  1/2,1/2,3/4 [0,0,0]
4  b  4/m..  0,0,0 [0,0,w]  0,0,1/2 [0,0,w]
4  a  422  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4mm1'
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0]  p 2mm1'
\[ a^* = b \quad b^* = c/2 \]
Origin at x,0,0

Along [1,1,0]  p₃ 2mm
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x-1/4,x+1/4,0
**Origin** at center (4/m' ) at 4/m'cc

**Asymmetric unit**  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

**Symmetry Operations**

For (0,0,0) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>1</td>
<td>(1,0,0)</td>
</tr>
<tr>
<td>(2)</td>
<td>2</td>
<td>(0,0,z) (2z,0,0,0)</td>
</tr>
<tr>
<td>(3)</td>
<td>4+</td>
<td>0,0,z (4z,0,0,0)</td>
</tr>
<tr>
<td>(4)</td>
<td>4-</td>
<td>0,0,z (4z,1,0,0)</td>
</tr>
<tr>
<td>(5)</td>
<td>2'</td>
<td>0,y,1/4 (2y,0,0,1/2)</td>
</tr>
<tr>
<td>(6)</td>
<td>2'</td>
<td>x,0,1/4 (2x,0,0,1/2)</td>
</tr>
<tr>
<td>(7)</td>
<td>2'</td>
<td>x,x,1/4 (2x,0,0,1/2)</td>
</tr>
<tr>
<td>(8)</td>
<td>2'</td>
<td>x,x,1/4 (2x,0,0,1/2)</td>
</tr>
<tr>
<td>(9)</td>
<td>3'</td>
<td>0,0,0 (1,0,0)</td>
</tr>
<tr>
<td>(10)</td>
<td>3'</td>
<td>m',x,y,0 (m',0,0,0)</td>
</tr>
<tr>
<td>(11)</td>
<td>3'</td>
<td>0,0,0 (m',0,0,0)</td>
</tr>
<tr>
<td>(12)</td>
<td>3'</td>
<td>0,0,0 (m',0,0,0)</td>
</tr>
<tr>
<td>(13)</td>
<td>c</td>
<td>(0,0,1/2) x,0,z (m,0,0,1/2)</td>
</tr>
<tr>
<td>(14)</td>
<td>c</td>
<td>(0,0,1/2) x,0,z (m,0,0,1/2)</td>
</tr>
<tr>
<td>(15)</td>
<td>c</td>
<td>(0,0,1/2) x,0,z (m,0,0,1/2)</td>
</tr>
<tr>
<td>(16)</td>
<td>c</td>
<td>(0,0,1/2) x,0,z (m,0,0,1/2)</td>
</tr>
</tbody>
</table>
Continued

For (1,0,0)' + set

(1) t'(1,0,0) (2) 2' 1/2,0,z (3) 4' 1/2,1/2,z (4) 4' 1/2,-1/2,z
(1) t'(1,0,0) (2) 2' 1/2,0,z (4) 1/2,-1/2,z

(5) 2 1/2,y,1/4 (2) 1,0,1/2 (3) 2 1/2,-1/2,0 (4) 1/2,1/2,0
(5) 2 1/2,y,1/4 (2) 1,0,1/2 (3) 2 1/2,-1/2,0 (4) 1/2,1/2,0

(9) T 1/2,0,0 (10) a 1,0,0 (11) 2 (1/2,1/2,0) x+1/2,x,1/4
(9) T 1/2,0,0 (10) a 1,0,0 (11) 2 (1/2,1/2,0) x+1/2,x,1/4

(13) n' (1,0,1/2) x,0,z (14) c' (0,0,1/2) 1/2,y,z
(13) n' (1,0,1/2) x,0,z (14) c' (0,0,1/2) 1/2,y,z

Generators selected (1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>16</th>
<th>m</th>
<th>m'..</th>
<th>(x,y,0) [u,v,0]</th>
<th>(x,y,1/2) [u,v,0]</th>
<th>(x,1/2,0) [u,v,0]</th>
<th>(x,0,1/2) [u,v,0]</th>
<th>(x,0,3/4) [u,v,0]</th>
<th>(x,3/4,0) [u,v,0]</th>
<th>(x,1/4,0) [u,v,0]</th>
<th>(x,1/4,3/4) [u,v,0]</th>
<th>(x,3/4,1/4) [u,v,0]</th>
<th>(x,1/4,1/4) [u,v,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>n</td>
<td>1</td>
<td>(x,y,z) [u,v,w]</td>
<td>(x,y,z+1/2) [u,v,w]</td>
<td>(x+1/2,y,z) [u,v,w]</td>
<td>(x+1/2,y,z+1/2) [u,v,w]</td>
<td>(x+1/2,y,z) [u,v,w]</td>
<td>(x+1/2,y,z+1/2) [u,v,w]</td>
<td>(x,y,z) [u,v,w]</td>
<td>(x+1/2,y,z) [u,v,w]</td>
<td>(x+1/2,y,z+1/2) [u,v,w]</td>
<td>(x,y,z) [u,v,w]</td>
</tr>
</tbody>
</table>

Coordinates

(0,0,0) + (1,0,0)' +

---

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<table>
<thead>
<tr>
<th>#</th>
<th>Symmetry</th>
<th>Special Projection</th>
<th>[u,v,0]</th>
<th>[v,u,0]</th>
<th>[v,u,0]</th>
<th>[v,u,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>e 2'/m'..</td>
<td>0,1/2,0 [u,v,0]</td>
<td>1/2,0,0 [v,u,0]</td>
<td>0,1/2,1/2 [u,v,0]</td>
<td>1/2,0,1/2 [v,u,0]</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>d 4'/m'..</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c 4'22'</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>b 4/m'..</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>a 42'2'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p, 4m'm'
  - \( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
  - Origin at 0,0,z

- **Along [1,0,0]**: p 2mm1'
  - \( \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}/2 \)
  - Origin at x,0,0

- **Along [1,1,0]**: p, 2mm
  - \( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)
  - Origin at x-1/4, x+1/4, 1/4
PP 4'/mcc'

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4/mmm1'

Tetragonal

PP 4'/m2/c2'/c'

Origin at center (4'/m) at 4'/mcc'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

For (0,0,0) + set

(1) 1

(2) 2 0,0,z
    (2z) 0,0,0

(3) 4' 0,0,z
    (4z) 0,0,0'

(4) 4' 0,0,z
    (4z) 0,0,0'

(5) 2 0,y,1/4
    (2y) 0,0,1/2

(6) 2 x,0,1/4
    (2x) 0,0,1/2

(7) 2' x,x,1/4
    (2xy) 0,0,1/2'

(8) 2' x,x,1/4
    (2xy) 0,0,1/2'

(9) 1 0,0,0
    (1) 0,0,0

(10) m x,y,0
     (mz) 0,0,0

(11) 4 0,0,z; 0,0,0
     (4z) 0,0,0'

(12) 4' 0,0,z; 0,0,0
     (4z) 0,0,0'

(13) c (0,0,1/2) x,0,z
     (mz) 0,0,1/2

(14) c (0,0,1/2) 0,y,z
     (mz) 0,0,1/2

(15) c' (0,0,1/2) x,x,z
     (mz) 0,0,1/2'

(16) c' (0,0,1/2) x,x,z
     (mz) 0,0,1/2'
Continued

For $(1,0,0)' +$ set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1)'(1,0,0)$</td>
<td>$(0,0,0) +$</td>
</tr>
<tr>
<td>$(1)(1,0,0)'$</td>
<td>$(1,0,0)' +$</td>
</tr>
<tr>
<td>$(2)' 1/2,0,z$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(2)(1,0,0)'$</td>
<td>$(1,0,0)$</td>
</tr>
<tr>
<td>$(3) 4'\ -1/2,1/2,z$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(4) 4'\ -1/2,1/2,z$</td>
<td>$(1,0,0)$</td>
</tr>
<tr>
<td>$(5) 2'/1/2,y,1/4$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(6) 2'(1,0,0)'\ x,0,1/4$</td>
<td>$(1,0,0)$</td>
</tr>
<tr>
<td>$(7) 2(1/2,1/2,0)'\ x+1/2,x,1/4$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(8) 2(1/2,-1/2,0)'\ x+1/2,x,1/4$</td>
<td>$(1,0,0)$</td>
</tr>
<tr>
<td>$(9) T'1/2,0,0$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(10) a'(1,0,0)'\ x,y,0$</td>
<td>$(1,0,0)$</td>
</tr>
<tr>
<td>$(11) 4'\ \ 1/2,-1/2,z; 1/2,-1/2,0$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(12) 4'\ \ 1/2,-1/2,z; 1/2,-1/2,0$</td>
<td>$(1,0,0)$</td>
</tr>
<tr>
<td>$(13) n'(1,0,1/2)'\ x,0,z$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(14) c'(0,0,1/2)'\ 1/2,y,z$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(15) n(1/2,-1/2,1/2)'\ x+1/2,x,z$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>$(16) n(1/2,1/2,1/2)'\ x+1/2,x,z$</td>
<td>$(0,0,0)$</td>
</tr>
</tbody>
</table>

Generators selected $(1); (1,0,0); (0,0,1); (2); (3); (5); (9).$

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>n</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>m</td>
<td>$(1,0,0)'$</td>
</tr>
<tr>
<td>16</td>
<td>i</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>j</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>i</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>h</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>g</td>
<td>$(0,0,0)$</td>
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<td>f</td>
<td>$(0,0,0)$</td>
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</tbody>
</table>

Positions

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<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>16</td>
<td>m</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>i</td>
<td>$(0,0,0)$</td>
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<tr>
<td>16</td>
<td>j</td>
<td>$(0,0,0)$</td>
</tr>
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<td>16</td>
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<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>h</td>
<td>$(0,0,0)$</td>
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<tr>
<td>16</td>
<td>g</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>f</td>
<td>$(0,0,0)$</td>
</tr>
</tbody>
</table>

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Symmetry of Special Projections

Along [0,0,1] p4mm1’
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p 2mm1’
\( a^* = b \quad b^* = c/2 \)
Origin at x,0,0

Along [1,1,0] p2a*, 2mm
\( a^* = (a + b)/2 \quad b^* = c/2 \)
Origin at x-1/4,x+1/4,0

8 e 2/m. 0.1/2,0 [0,0,0] 1/2,0,0 [0,0,0] 0.1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]
4 d 4/m. 1/2,1/2,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]
4 c 422 1/2,1/2,1/4 [0,0,0] 1/2,1/2,3/4 [0,0,0]
4 b 4/m. 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]
4 a 422 0,0,1/4 [0,0,0] 0,0,3/4 [0,0,0]
Origin at center (4'/m') at 4'/m'cc'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

1. 1
   (1|0,0,0)

2. 2 0,0,z
   (2_2,0,0,0)

3. 4⁺ 0,0,z
   (4_2,0,0,0')

5. 0,0,1/4
   (2,0,0,1/2')

6. 2⁺ x,0,1/4
   (2_x,0,0,1/2')

7. 2 x,x,1/4
   (2_xy,0,0,1/2)

8. 2 x,x,1/4
   (2_xy,0,0,1/2)

9. 0,0,0
   (1|0,0,0')

10. m' x,y,0
    (m_2,0,0,0')

11. 4⁺ 0,0,z; 0,0,0
    (4_2,0,0,0)

12. 4⁺ 0,0,z; 0,0,0
    (4_2,0,0,0)

13. c (0,0,1/2) x,0,z
    (m_2,0,0,1/2)

14. c (0,0,1/2) 0,y,z
    (m_2,0,0,1/2)

15. c' (0,0,1/2) x,x,z
    (m_x,0,0,1/2')

16. c' (0,0,1/2) x,x,z
    (m_x,0,0,1/2')
For $(1,0,0)' + \text{set}$

(1) $t'(1,0,0)$
(2) $2' 1/2,0,z$
(3) $4' -1/2,1/2,z$
(4) $4' 1/2,-1/2,z$

(5) $2 1/2,y,1/4$
(2) $1,0,1/2$

(9) $1/2,0,0$

(13) $n'(1,0,1/2) x,0,z$

Generators selected (1); $t'(1,0,0)$; $t'(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 n 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) $\bar{x},y,z [\bar{u},v,w]$</td>
</tr>
<tr>
<td>16 m m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>$\bar{x},\bar{y},0 [\bar{u},\bar{v},0]$</td>
</tr>
<tr>
<td>16 l .2.</td>
<td>x,1/2,1/4 [u,0,0]</td>
<td>$\bar{x},1/2,1/4 [\bar{u},0,0]$</td>
</tr>
<tr>
<td>16 k .2'.</td>
<td>x,0,1/4 [0,v,w]</td>
<td>$\bar{x},0,1/4 [\bar{0},v,w]$</td>
</tr>
<tr>
<td>16 j .2</td>
<td>x,x,1/4 [u,u,0]</td>
<td>$\bar{x},x,1/4 [\bar{u},u,0]$</td>
</tr>
<tr>
<td>16 i .2'..</td>
<td>x,x,3/4 [u,u,0]</td>
<td>$\bar{x},x,3/4 [\bar{u},u,0]$</td>
</tr>
<tr>
<td>8 h 4..</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>$1/2,1/2,z+1/2 [0,0,w]$</td>
</tr>
<tr>
<td>8 g 4'..</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>8 f 2'2'..</td>
<td>0,1/2,1/4 [u,0,0]</td>
<td>$1/2,0,1/4 [0,u,0]$</td>
</tr>
<tr>
<td></td>
<td></td>
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</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>8</td>
<td>e</td>
<td>2/m'..</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>4/m'..</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>422</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>4'/m'..</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>4'2'2</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] \( p\_p, 4m'm' \)

- \( a^* = a \)
- \( b^* = b \)

Origin at 1/2,1/2,z

Along [1,0,0] \( p\, 2mm1' \)

- \( a^* = b \)
- \( b^* = c/2 \)

Origin at x,0,0

Along [1,1,0] \( p\_2\, 2m'm' \)

- \( a^* = (-a + b)/2 \)
- \( b^* = c/2 \)

Origin at x,x,0
Origin at 422 at 4/n22/g, at -1/4, -1/4, 0 from center (2/m)

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

1. 1
   (1 | 0,0,0)

2. 2   0,0,z
      (2 | 0,0,0)

3. 4+  0,0,z
      (4 | 0,0,0)

4. 4-  0,0,z
      (4- | 0,0,0)

5. 2   0,y,0
      (2y | 0,0,0)

6. 2   x,0,0
      (2x | 0,0,0)

7. 2   x,x,0
      (2x | 0,0,0)

8. 2   x,0,z
      (2xz | 0,0,0)

9. 1/4,1/4,0
   (1 | 1/2,1/2,0)

10. n   1/2,1/2,0
     (m | 1/2,1/2,0)

11. 4+  1/2,0,z; 1/2,0,0
     (2 | 1/2,1/2,0)

12. 4-  0,1/2,z; 0,1/2,0
     (2- | 1/2,1/2,0)

13. a   1/2,0,0
     (m | 1/2,1/2,0)

14. b   0,1/2,0
     (m | 1/2,1/2,0)

15. m   x+1/2,0,z
     (nxy | 1/2,1/2,0)

16. g   1/2,1/2,0
     (nxy | 1/2,1/2,0)
**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 n 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z ([u,v,w])</td>
<td>(2) x+1/2, y+1/2, (\bar{z}) ([u,v,w])</td>
<td>(3) x, y, z ([\bar{u}, \bar{v}, \bar{w}])</td>
<td>(4) x, y, z ([\bar{v}, \bar{u}, \bar{w}])</td>
</tr>
<tr>
<td>(5) x, y, z ([u,v,w])</td>
<td>(6) x, y, z ([u,v,w])</td>
<td>(7) y, x, z ([v,u,w])</td>
<td>(8) y, x, z ([v,u,w])</td>
</tr>
<tr>
<td>(9) x+1/2, y+1/2, (\bar{z}) ([u,v,w])</td>
<td>(10) x+1/2, y+1/2, (\bar{z}) ([u,v,w])</td>
<td>(11) y+1/2, (\bar{x}) +1/2, (\bar{z}) ([v,u,w])</td>
<td>(12) (y) +1/2, (x) +1/2, (\bar{z}) ([v,u,w])</td>
</tr>
<tr>
<td>(13) x+1/2, y+1/2, (\bar{z}) ([u,v,w])</td>
<td>(14) x+1/2, y+1/2, (\bar{z}) ([u,v,w])</td>
<td>(15) y+1/2, (\bar{x}) +1/2, (\bar{z}) ([v,u,w])</td>
<td>(16) y+1/2, (x) +1/2, (\bar{z}) ([v,u,w])</td>
</tr>
</tbody>
</table>

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).
Symmetry of Special Projections

Along [0,0,1]  \( \rho_p \)  4m'm'
\( \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \)
\( \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \)
Origin at 0,0,z

Along [1,0,0]  \( \rho_{2a} \)  2m'm'
\( \mathbf{a}^* = \mathbf{b}/2 \)
\( \mathbf{b}^* = \mathbf{c} \)
Origin at x,0,0

Along [1,1,0]  \( \rho \)  2mm1'
\( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \)
\( \mathbf{b}^* = \mathbf{c} \)
Origin at x,x,0
Origin at 4221' at 4/n22/g1', at -1/4,-1/4,0 from center (2/m1')

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

For 1 + set

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(22) 0,0,0

(3) 4+ 0,0,z
(42) 0,0,0

(4) 4- 0,0,z
(42) 0,0,0

(5) 2 0,y,0
(22) 0,0,0

(6) 2 x,0,0
(22) 0,0,0

(7) 2 x,x,0
(22) 0,0,0

(8) 2 x,x,0
(22) 0,0,0

(9) 1/4,1/4,0

(1) 1/2,1/2,0

(10) n (1/2,1/2,0) x,y,0
(m2) 1/2,1/2,0

(11) 4+ 1/2,0,z; 1/2,0,0
(42) 1/2,1/2,0

(12) 4- 0,1/2,z; 0,1/2,0
(42) 1/2,1/2,0

(13) a (1/2,0,0) x,1/4,z
(m2) 1/2,1/2,0

(14) b (0,1/2,0) 1/4,y,z
(m2) 1/2,1/2,0

(15) m x+1/2, y,z
(m2) 1/2,1/2,0

(16) g (1/2,1/2,0) x,x,z
(m2) 1/2,1/2,0

125.2.1032 - 1 - 2094
For 1' + set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1'</td>
<td>(1) $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)</td>
<td>16</td>
<td>n</td>
<td>11'</td>
</tr>
<tr>
<td>1'</td>
<td>x,y,z [0,0,0]</td>
<td>8</td>
<td>m</td>
<td>..m1'</td>
</tr>
<tr>
<td></td>
<td>x,y,z [0,0,0]</td>
<td>8</td>
<td>i</td>
<td>..21'</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [0,0,0]</td>
<td>8</td>
<td>j</td>
<td>.21'</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [0,0,0]</td>
<td>8</td>
<td>k</td>
<td>.21'</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [0,0,0]</td>
<td>8</td>
<td>l</td>
<td>.21'</td>
</tr>
<tr>
<td>1'</td>
<td>x,x+1/2,z [0,0,0]</td>
<td>4</td>
<td>h</td>
<td>2.mm1'</td>
</tr>
</tbody>
</table>

Generators selected:
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.
### Symmetry of Special Projections

Along $[0,0,1]$  \( p4mm1' \)

- \( a^* = (a - b)/2 \)
- \( b^* = (a + b)/2 \)

Origin at 0,0,z

Along $[1,0,0]$  \( p2mm1' \)

- \( a^* = b/2 \)
- \( b^* = c \)

Origin at x,0,0

Along $[1,1,0]$  \( p2mm1' \)

- \( a^* = -(a + b)/2 \)
- \( b^* = c \)

Origin at x,x,0

---

<table>
<thead>
<tr>
<th>4</th>
<th>g</th>
<th>4..1'</th>
<th>0,0,z [0,0,0]</th>
<th>0,0,z [0,0,0]</th>
<th>1/2,1/2,z [0,0,0]</th>
<th>1/2,1/2,z [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>f</td>
<td>..2/m1'</td>
<td>1/4,1/4,1/2 [0,0,0]</td>
<td>3/4,3/4,1/2 [0,0,0]</td>
<td>3/4,1/4,1/2 [0,0,0]</td>
<td>1/4,3/4,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>..2/m1'</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,3/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td>1/4,3/4,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>\overline{4}2m1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>\overline{4}2m1'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4221'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4221'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at $42'2'$ at $4/n'2'2'/g$, at $-1/4,-1/4,0$ from center ( $2'/m$ )

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

**Symmetry Operations**

1. $1$
2. $2' \quad 0,0,z$
3. $4' \quad 0,0,z$
4. $4' \quad 0,0,z$
5. $2' \quad 0,y,0$
6. $2' \quad x,0,0$
7. $2' \quad x,x,0$
8. $2' \quad x,x,0$
9. $3' \quad 1/4,1/4,0$
10. $3' \quad 1/4,1/4,0$
11. $4' \quad 1/2,0,z$
12. $4' \quad 1/2,0,z$
13. $a \quad (1/2,0,0)
14. $b \quad (0,1/2,0)$
15. $m \quad x+1/2,\bar{x},z$
16. $g \quad (1/2,1/2,0)$
Continued

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 n 1</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(9) x+1/2,y+1/2,z [u,v,w]</td>
<td>(10) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(13) x+1/2,y+1/2,z [u,v,w]</td>
<td>(14) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 8 m ..m | x,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] |
| 8 l .2'. | x,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] |
| 8 k .2'. | x,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] |
| 8 j .2' | x,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] | x+1/2,x+1/2,z [u,u,0] |

| 4 h 2.mm | 0,1/2,z [0,0,0] | 1/2,0,2 [0,0,0] | 0,1/2,z [0,0,0] | 1/2,0,2 [0,0,0] |
| 4 g 4.. | 0,0,z [0,0,0] | 0,0,z [0,0,0] | 1/2,1/2,z [0,0,0] | 1/2,1/2,z [0,0,0] |
| 4 f .2'm | 1,4,1/4,1/2 [0,0,0] | 3/4,3/4,1/2 [0,0,0] | 3/4,3/4,1/2 [0,0,0] | 1/4,3/4,1/2 [0,0,0] |
| 4 e .2'm | 1,4,1/4,0 [0,0,0] | 3/4,3/4,0 [0,0,0] | 3/4,3/4,0 [0,0,0] | 1/4,3/4,0 [0,0,0] |

| 2 d 42'2m | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |
| 2 c 42'2m | 0,1/2,0 [0,0,0] | 1/2,0,0 [0,0,0] |
| 2 b 42'2' | 0,0,1/2 [0,0,w] | 1/2,1/2,1/2 [0,0,w] |
| 2 a 42'2' | 0,0,0 [0,0,w] | 1/2,1/2,0 [0,0,w] |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>p4mm</th>
<th>p 2m'm'</th>
<th>p 2mm'1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$a^* = (a - b)/2$</td>
<td>$b^* = (a + b)/2$</td>
<td>$a^* = b/2$</td>
<td>$b^* = c$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$a^* = (-a + b)/2$</td>
<td>$b^* = c$</td>
</tr>
</tbody>
</table>

Origin at x,0,0

Origin at x,x,0
Origin at 4'2'2 at 4'/n2'2/g, at -1/4,-1/4,0 from center (2/m)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x \]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2_z \mid 0,0,0) \\
(3) & \quad 4^+ \quad 0,0,z \\
& \quad (4_z \mid 0,0,0)' \\
(4) & \quad 4^- \quad 0,0,z \\
& \quad (4_z^{-1} \mid 0,0,0)' \\
(5) & \quad 2' \quad 0,y,0 \\
& \quad (2_y \mid 0,0,0)' \\
(6) & \quad 2' \quad x,0,0 \\
& \quad (2_x \mid 0,0,0)' \\
(7) & \quad 2 \quad x,x,0 \\
& \quad (2_{xy} \mid 0,0,0) \\
(8) & \quad 2 \quad x,x,0 \\
& \quad (2_{xy} \mid 0,0,0) \\
(9) & \quad \overline{1} \quad 1/4,1/4,0 \\
& \quad (1 \mid 1/2,1/2,0) \\
(10) & \quad n \quad (1/2,1/2,0) \\
& \quad x,y,0 \\
& \quad (m_z \mid 1/2,1/2,0) \\
(11) & \quad 4^+ \quad 1/2,0,z; 1/2,0,0 \\
& \quad (4_z \mid 1/2,1/2,0) \\
& \quad 0,1/2,z; 0,1/2,0 \\
& \quad (4_z^{-1} \mid 1/2,1/2,0)' \\
(12) & \quad a' \quad (1/2,2,0) \\
& \quad x,1/4,z \\
& \quad (m_y \mid 1/2,1/2,0)' \\
(13) & \quad b' \quad (0,1/2,0) \\
& \quad 1/4,y,z \\
& \quad (m_x \mid 1/2,1/2,0)' \\
(14) & \quad m \quad x+1/2,x,z \\
& \quad (m_{xy} \mid 1/2,1/2,0) \\
(15) & \quad g \quad (1/2,1/2,0) \\
& \quad x,x,z \\
& \quad (m_{xy} \mid 1/2,1/2,0)
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site symmetry</th>
</tr>
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<tbody>
<tr>
<td>16</td>
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<td>m</td>
<td>..m</td>
</tr>
<tr>
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<td>.2'</td>
</tr>
<tr>
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<td>k</td>
<td>.2'</td>
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<tr>
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<td>f</td>
<td>..2/m</td>
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<td>..2/m</td>
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<td>4'2'm</td>
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<td>4'2'm</td>
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</tr>
<tr>
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</table>

Coordinates

<table>
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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>(5) x+1/2,x+1/2,1/2 [u,u,0]</td>
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<tr>
<td>(9) x+1/2,x+1/2,1/2 [u,u,0]</td>
</tr>
<tr>
<td>(13) x+1/2,x+1/2,1/2 [u,u,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p'\text{4mm}
\begin{align*}
a^* &= \frac{a - b}{2} \quad b^* &= \frac{a + b}{2} \\
\text{Origin at 1/2,0,}z &
\end{align*}

Along [1,0,0] p_{2a'}^* 2'mm'
\begin{align*}
a^* &= -c \quad b^* &= \frac{b}{2} \\
\text{Origin at x,0,} &
\end{align*}

Along [1,1,0] p 2'mm'
\begin{align*}
a^* &= -c \quad b^* &= \frac{(-a + b)}{2} \\
\text{Origin at x,x,} &
\end{align*}
Origin at 4'22' at 4'/n22'/g', at -1/4,-1/4,0 from center (2'/m')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x \]

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2' 0,0,z
(2_z | 0,0,0)

(3) 4' 0,0,z
(4_z | 0,0,0')

(4) 4' 0,0,z
(4_z | 0,0,0')

(5) 2' 0,y,0
(2_y | 0,0,0)

(6) 2' x,0,0
(2_x | 0,0,0)

(7) 2' x,x,0
(2_x | 0,0,0')

(8) 2' x,x,0
(2_x | 0,0,0')

(9) \overline{1} 1/4,1/4,0
(1 | 1/2,1/2,0)

(10) n (1/2,1/2,0) x,y,0
(m_x | 1/2,1/2,0)

(11) 4' 1/2,0,z; 1/2,0,0
(4_z | 1/2,1/2,0')

(12) 4' 0,1/2,z; 0,1/2,0
(4_z | 1/2,1/2,0')

(13) a (1/2,0,0) x,1/4,z
(m_y | 1/2,1/2,0)

(14) b (0,1/2,0) 1/4,y,z
(m_z | 1/2,1/2,0)

(15) m' x+1/2,x,z
(m_x | 1/2,1/2,0')

(16) g' (1/2,1/2,0) x,x,z
(m_y | 1/2,1/2,0')
# Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

## Positions

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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tr>
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<td>[0,0,0]</td>
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<th>a</th>
<th>4'22'</th>
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<tr>
<td>0,0,0</td>
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<tr>
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125.5.1035 - 2 - 2104
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
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<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>$p_{gm}$ 4m'm'</td>
<td>Origin at $1/2,0,0$</td>
</tr>
<tr>
<td>$a^* = (a - b)/2$</td>
<td>$b^* = (a + b)/2$</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>$p_{2/a} 2m'm'$</td>
<td>Origin at $x,0,0$</td>
</tr>
<tr>
<td>$a^* = b/2$</td>
<td>$b^* = c$</td>
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</tr>
<tr>
<td>Along [1,1,0]</td>
<td>$p_{2/m}m'$</td>
<td>Origin at $x,x,0$</td>
</tr>
<tr>
<td>$a^* = -c$</td>
<td>$b^* = (-a + b)/2$</td>
<td></td>
</tr>
</tbody>
</table>
P4'/n'b'm
125.6.1036

P4'/n'2/b'2'/m
Tetragonal

Origin at 4'22' at 4'/n'22'/g, at -1/4,-1/4,0 from center (2'/m)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

(1) 1
(1) 0,0,0
(2) 2 0,0,z
(2) z 0,0,0
(3) 4 + 0,0,z
(3) 4+z 0,0,0'
(4) 4 - 0,0,z
(4) 4+z 0,0,0'

(5) 2 0,y,0
(5) 0,y,0
(6) 2 x,0,0
(6) x 0,0,0
(7) 2' x,x,0
(7) x,x,0
(2) y x,0
(2) x y,0

(9) 1/4,1/4,0
(1) 1/2,1/2,0
(10) n' (1/2,1/2,0) x,y,0
(10) m 1/2,1/2,0
(11) 4+ 1/2,0,z; 1/2,0,0
(11) 4+z 1/2,1/2,0
(12) 4- 0,1/2,z; 0,1/2,0
(12) 4- 1/2,1/2,0

(13) a' (1/2,0,0) x,1/4,z
(13) m 1/2,1/2,0
(14) b' (0,1/2,0) 1/4,y,z
(14) m 1/2,1/2,0
(15) m x+1/2,x,z
(15) m 1/2,1/2,0
(16) g (1/2,1/2,0) x,x,z
(16) m 1/2,1/2,0

125.6.1036 - 1 - 2106
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Coordinates</th>
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<tbody>
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<tr>
<td>(2) x, x, z [u, v, w]</td>
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</tr>
<tr>
<td>(3) y, x, z [v, u, w]</td>
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<td>(4) y, x, z [v, u, w]</td>
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<td>(7) y, x, z [v, u, w]</td>
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<tr>
<td>(8) y, x, z [v, u, w]</td>
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<tr>
<td>(9) x+1/2, y+1/2, z  [u, v, w]</td>
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<tr>
<td>(10) x+1/2, y+1/2, z [u, v, w]</td>
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<td>0, 1/2, z [0, 0, 0]</td>
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<td>0, 1/2, z [0, 0, 0]</td>
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<table>
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<tr>
<th>Coordinates</th>
<th>2 d 42m</th>
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<tr>
<td>0, 1/2, 1/2 [0, 0, 0]</td>
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<td>1/2, 0, 1/2 [0, 0, 0]</td>
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<tr>
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<th>2 c 42m</th>
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<tr>
<td>0, 1/2, 0 [0, 0, 0]</td>
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<table>
<thead>
<tr>
<th>Coordinates</th>
<th>2 b 4'22'</th>
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<tr>
<td>0, 0, 1/2 [0, 0, 0]</td>
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<td>1/2, 1/2, 1/2 [0, 0, 0]</td>
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<thead>
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<th>Coordinates</th>
<th>2 a 4'22'</th>
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</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>1/2, 1/2, 0 [0, 0, 0]</td>
<td></td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p4'mm'
\[ a^* = \frac{a - b}{2}, \quad b^* = \frac{a + b}{2} \]
Origin at 0,0,z

Along [1,0,0] p 2m'm'
\[ a^* = \frac{b}{2}, \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p 2mm1'
\[ a^* = \frac{-a + b}{2}, \quad b^* = c \]
Origin at x,x,0
Origin at 42'2' at 4/n2'2'/g', at -1/4,-1/4,0 from center (2'm')

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

(1) 1
(1 | 0,0,0)

(5) 2'
0,y,0
(2'y | 0,0,0')

(9) 1/4,1/4,0
(1 | 1/2,1/2,0)

(13) a'
(1/2,0,0)
(m' | 1/2,1/2,0')

(2) 2
0,0,z
(2z | 0,0,0)

(6) 2'
x,0,0
(2z | 0,0,0')

(10) n
(1/2,1/2,0)
x,y,0
(mz | 1/2,1/2,0)

(14) b'
(0,1/2,0)
1/4,y,z
(mx | 1/2,1/2,0')

(3) 4
0,0,z
(4z | 0,0,0)

(7) 2'
x,x,0
(2y | 0,0,0')

(11) 4
1/2,0,z; 1/2,0,0
(4z | 1/2,1/2,0)

(15) m'
x+1/2,x,z
(mx | 1/2,1/2,0')

(4) 4'
0,0,z
(4z | 0,0,0)

(8) 2'
x,x,0
(2y | 0,0,0')

(12) 4
0,1/2,z; 0,1/2,0
(4z | 1/2,1/2,0)

(16) g'
(1/2,1/2,0)
x,x,z
(mx | 1/2,1/2,0)
Generators selected

(1) t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>n</td>
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<tr>
<td>(1) x,y,z [u,v,w]</td>
<td></td>
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<td>x,x+1/2,z [u,u,w]</td>
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<tr>
<td>(2) x,y,z [u,v,w]</td>
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<td>x+1/2,x,z [u,u,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>x+1/2,x,z [u,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<td>x+1/2,x,z [u,u,w]</td>
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<tr>
<td>(5) x,y,z [u,v,w]</td>
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<td>(6) x,y,z [u,v,w]</td>
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<td>x+1/2,x,z [u,u,w]</td>
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<td>(7) y,x,z [v,u,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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<td>x+1/2,x,z [u,u,w]</td>
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<td>(9) x+1/2,y+1/2,z [u,v,w]</td>
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<td>x+1/2,x+1/2,z [v,u,w]</td>
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<tr>
<td>(10) x+1/2,y+1/2,z [u,v,w]</td>
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<td>x+1/2,x+1/2,z [v,u,w]</td>
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<td>(11) y+1/2,x+1/2,z [v,u,w]</td>
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<td>x+1/2,x+1/2,z [v,u,w]</td>
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<td>(12) y+1/2,x+1/2,z [v,u,w]</td>
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<td>x+1/2,x+1/2,z [v,u,w]</td>
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<td>(15) y+1/2,x+1/2,z [v,u,w]</td>
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<td>8</td>
<td>i   .2'</td>
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<td>(1) x,y,z [u,v,w]</td>
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</table>

Continued 125.7.1037 P4/nb'm'
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Transformation</th>
<th>Origin</th>
</tr>
</thead>
</table>
| Along [0,0,1]   | p' 4mm   | $a^* = (a - b)/2$  
$\begin{align*}
a^* &= (a - b)/2 \\
b^* &= (a + b)/2 \\
\end{align*}$ | Origin at 0,0,z |
| Along [1,0,0]   | p 2m'm'  | $a^* = b/2$     
$\begin{align*}
a^* &= b/2 \\
b^* &= c \\
\end{align*}$ | Origin at x,0,0 |
| Along [1,1,0]   | p 2'm'm' | $a^* = -c$     
$\begin{align*}
a^* &= -c \\
b^* &= (-a + b)/2 \\
\end{align*}$ | Origin at x,x,0 |
**Tetragonal**

**Symmetry Operations**

1. 1
   
   (1) 1
   
   (1 0 0 0)

2. 2' 0,0,z
   
   (2 0 0 0)

3. 4' 0,0,z
   
   (4 0 0 0)

4. -4' 0,0,z
   
   (4 0 0 0)

5. 2' 0,y,0
   
   (2 0 0 0)

6. 2' x,0,0
   
   (2 0 0 0)

7. 2' x,x,0
   
   (2 0 0 0)

8. 2' x,x,0
   
   (2 0 0 0)

9. 2' 0,y,0
   
   (2 0 0 0)

10. 2' x,0,0
    
    (2 0 0 0)

11. 2' x,x,0
    
    (2 0 0 0)

12. 2' x,x,0
    
    (2 0 0 0)

13. 2' 0,z,0
    
    (2 0 0 0)

14. 2' x,0,0
    
    (2 0 0 0)

15. 2' x,x,0
    
    (2 0 0 0)

16. 2' x,x,0
    
    (2 0 0 0)

**Origin**

at 4'/2'/2 at 4'/n'2'/2/g', at -1/4,-1/4,0 from center (2/m')

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

16 n 1

(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y,x,z [v,u,w]  (4) y,x,z [v,u,w]
(5) x,y,z [u,v,w]  (6) x,y,z [u,v,w]  (7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]
(9) x+1/2,y+1/2,z [u,v,w]  (10) x+1/2,y+1/2,z [u,v,w]  (11) y+1/2,x+1/2,z [v,u,w]  (12) y+1/2,x+1/2,z [v,u,w]
(13) x+1/2,y+1/2,z [u,v,w]  (14) x+1/2,y+1/2,z [u,v,w]  (15) y+1/2,x+1/2,z [v,u,w]  (16) y+1/2,x+1/2,z [v,u,w]

8 m ..m'

x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x+1/2,x,z [u,u,w]  x+1/2,x,z [u,u,w]

x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x+1/2,x,z [u,u,w]  x+1/2,x,z [u,u,w]

8 l .2'.

x,0,1/2 [0,v,w]  x,0,1/2 [0,v,w]  0,x,1/2 [v,0,w]  0,x,1/2 [v,0,w]

x+1/2,1/2,1/2 [0,v,w]  x+1/2,1/2,1/2 [0,v,w]  1/2,x+1/2,1/2 [v,0,w]  1/2,x+1/2,1/2 [v,0,w]

8 k .2'.

x,0,0 [0,v,w]  x,0,0 [0,v,w]  0,x,0 [v,0,w]  0,x,0 [v,0,w]

x+1/2,1/2,0 [0,v,w]  x+1/2,1/2,0 [0,v,w]  1/2,x+1/2,0 [v,0,w]  1/2,x+1/2,0 [v,0,w]

8 j .2

x,x,1/2 [u,u,0]  x,x,1/2 [u,u,0]  x,x,1/2 [u,u,0]  x,x,1/2 [u,u,0]

x+1/2,x+1/2,1/2 [u,u,0]+x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]

8 i .2

x,x,0 [u,u,0]  x,x,0 [u,u,0]  x,x,0 [u,u,0]  x,x,0 [u,u,0]

x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]

4 h 2.m'm'

0,1/2,z [0,0,w]  1/2,0,z [0,0,w]  0,1/2,z [0,0,w]  1/2,0,z [0,0,w]

4 g 4'..

0,0,z [0,0,0]  0,0,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]

4 f .2m'

1/4,1/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]

4 e .2m'

1/4,1/4,0 [0,0,0]  3/4,3/4,0 [0,0,0]  3/4,3/4,0 [0,0,0]  1/4,3/4,0 [0,0,0]

2 d 4'2m'

0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,w]  1/2,0,1/2 [0,0,0]  0,1/2,1/2 [0,0,w]

2 c 4'2m'

0,1/2,0 [0,0,0]  1/2,0,0 [0,0,w]  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,w]

2 b 4'2'

0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  0,0,1/2 [0,0,0]

2 a 4'2'

0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  0,0,0 [0,0,0]
## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Axis</th>
<th>Transformation</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>p4'm'm</td>
<td>[0,0,1]</td>
<td>$a^* = \frac{(a - b)}{2}$, $b^* = \frac{(a + b)}{2}$</td>
<td>0,0,z</td>
</tr>
<tr>
<td>p2a'-2mm</td>
<td>[1,0,0]</td>
<td>$a^* = \frac{b}{2}$, $b^* = c$</td>
<td>x,1/4,0</td>
</tr>
<tr>
<td>p 2m'm'</td>
<td>[1,1,0]</td>
<td>$a^* = \frac{(-a + b)}{2}$, $b^* = c$</td>
<td>x,x,0</td>
</tr>
</tbody>
</table>
**P4/n'b'm'**

**Origin**

at 422 at 4/n'22/g', at -1/4, -1/4, 0 from center (2/m')

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

**Symmetry Operations**

1. 1
   
   (1) 1
   
   (2) 2 0,0,z
   
   (3) 4+ 0,0,z
   
   (4) 4 0,0,z
   
   (5) 2 0,y,0
   
   (6) 2 x,0,0
   
   (7) 2 x,x,0
   
   (8) 2 x,x,0
   
   (9) 1/4,1/4,0
   
   (10) 1/2,1/2,0
   
   (11) 1/2,1/2,0
   
   (12) 1/2,1/2,0
   
   (13) 1/4,1/4,0
   
   (14) 1/2,1/2,0
   
   (15) 1/2,1/2,0
   
   (16) 1/2,1/2,0

125.9.1039 - 1 - 2115
### Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
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<tr>
<th>Generator</th>
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<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2)</td>
<td>x,y,z [u,v,w]</td>
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<td>y,x,z [v,u,w]</td>
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<td>y,x,z [v,u,w]</td>
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<td>x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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<td>(8)</td>
<td>y,x,z [v,u,w]</td>
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<td>(9)</td>
<td>x+1/2,y+1/2,z [u,v,w]</td>
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<td>(14)</td>
<td>x+1/2,y+1/2,z [u,v,w]</td>
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<td>(15)</td>
<td>y+1/2,x+1/2,z [v,u,w]</td>
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<tr>
<td>(16)</td>
<td>y+1/2,x+1/2,z [v,u,w]</td>
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<td>(18)</td>
<td>x+1/2,y+1/2,z [u,v,w]</td>
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<td>(19)</td>
<td>y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td>(20)</td>
<td>y+1/2,x+1/2,z [v,u,w]</td>
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### Coordinates

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<td>x+1/2,z [v,0]</td>
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<td>x+1/2,z [u,0]</td>
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<tr>
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<td>x+1/2,z [v,0]</td>
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</tr>
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<td>x+1/2,z [v,0]</td>
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<td>x+1/2,z [v,0]</td>
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<td>(20)</td>
<td>x+1/2,z [v,0]</td>
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</table>

### Additional Information

- **Continued:** 125.9.1039 P4/n'b'm'
- **Multiplicities:**...
- **Wyckoff letters:**...
- **Site Symmetry:**...
Symmetry of Special Projections

Along [0,0,1] \text{ p4m'}
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] \text{ p2m'}
\[ a^* = b/2 \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] \text{ p2m'}
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,0
P2c 4/nbm

4/mmm1'

Tetragonal

125.10.1040

P2c 4/n2/b2/m

125.10.1040 - 1 - 2118
Origin at 422 at 4/n22/g, at -1/4,-1/4,0 from center (2/m)

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)
(2) 2 0,0,z (2z|0,0,0)
(3) 4* 0,0,z (4z|0,0,0)
(4) 4' 0,0,z (4z'|0,0,0)
(5) 2 0,y,0 (2z|0,0,0)
(6) 2 x,0,0 (2z|0,0,0)
(7) 2 x,x,0 (2xy|0,0,0)
(8) 2 x,0,0 (2xy|0,0,0)
(9) T 1/4,1/4,0 (1|1/2,1/2,0)
(10) n (1/2,1/2,0) x,y,0 (11) 4*+ 1/2,0,z; 1/2,0,0 (4z|1/2,1/2,0)
(12) 4* 1/2,0; 0,1/2,0 (4z|1/2,1/2,0)
(13) a (1/2,0,0) x,1/4,z (m_1|1/2,1/2,0)
(14) b (0,1/2,0) 1/4,y,z (m_1|1/2,1/2,0)
(15) m x+1/2,x,z (m_1y|1/2,1/2,0)
(16) g (1/2,1/2,0) x,x,z (m_1y|1/2,1/2,0)

For (0,0,1)' + set

(1) t' (0,0,1) (1|0,0,1)
(2) 2' (0,0,1) 0,0,z (2z|0,0,0)'
(3) 4'*(0,0,1) 0,0,z (4z|0,0,0)'
(4) 4'*(0,0,1) 0,0,z (4z'|0,0,0)'
(5) 2' 0,y,1/2 (2z|0,0,1)'
(6) 2' x,0,1/2 (2z|0,0,1)'
(7) 2' x,x,1/2 (2xy|0,0,1)'
(8) 2' x,x,1/2 (2xy|0,0,1)'
(9) T' 1/4,1/4,1/2 (1|1/2,1/2,1)
(10) n' (1/2,1/2,0) x,y,1/2 (11) 4*'-1/2,0,z; 1/2,0,1/2 (4z|1/2,1/2,1)'
(12) 4*-0,1/2,0; 0,1/2,1/2 (4z'|1/2,1/2,1)'
(13) n' (1/2,0,1) x,1/4,z (m_1|1/2,1/2,1)'
(14) n' (0,1/2,1) 1/4,y,z (m_1|1/2,1/2,1)'
(15) c' (0,0,1) x+1/2,x,z (m_1y|1/2,1/2,1)'
(16) n' (1/2,1/2,1) x,x,z (m_1y|1/2,1/2,1)'

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

32 n 1

(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w]
(5) x,y,z [u,v,w] (6) x,y,z [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w]
(9) x+1/2,y+1/2,z [u,v,w] (10) x+1/2,y+1/2,z [u,v,w] (11) y+1/2,x+1/2,z [v,u,w] (12) y+1/2,x+1/2,z [v,u,w]
(13) x+1/2,y+1/2,z [u,v,w] (14) x+1/2,y+1/2,z [u,v,w] (15) y+1/2,x+1/2,z [v,u,w] (16) y+1/2,x+1/2,z [v,u,w]

16 m ..m x,x+1/2,z [u,u,0] x,x+1/2,z [u,u,0] x,x+1/2,z [u,u,0] x,x+1/2,z [u,u,0]
 x+1/2,x,z [u,u,0] x+1/2,x,z [u,u,0] x+1/2,x,z [u,u,0] x+1/2,x,z [u,u,0]
16  l  .2'.  x,0,1/2 [0,v,w]  \bar{x},0,1/2 [\bar{0},\bar{v},\bar{w}]  0,x,1/2 [v,0,w]  0,\bar{x},1/2 [\bar{v},0,\bar{w}]
\bar{x}+1/2,1/2,1/2 [0,\bar{v},\bar{w}]  x+1/2,1/2,1/2 [0,v,w]  1/2,\bar{x}+1/2,1/2 [\bar{v},0,\bar{w}]  1/2,x+1/2,1/2 [v,0,w]
16  k  .2.  x,0,0 [u,0,0]  \bar{x},0,0 [\bar{u},0,0]  0,x,0 [0,u,0]  0,\bar{x},0 [0,\bar{u},0]
\bar{x}+1/2,1/2,0 [u,0,0]  x+1/2,1/2,0 [u,0,0]  1/2,\bar{x}+1/2,0 [0,u,0]  1/2,x+1/2,0 [0,\bar{u},0]
16  j  ..2'  x,x,1/2 [u,u,w]  \bar{x},x,1/2 [\bar{u},\bar{u},w]  x,x,1/2 [0,0,w]  x,x,1/2 [u,\bar{u},w]
\bar{x}+1/2,x+1/2,1/2 [u,\bar{u},w]  x+1/2,x+1/2,1/2 [u,u,w]  x+1/2,\bar{x}+1/2,1/2 [0,0,0]  x+1/2,\bar{x}+1/2,1/2 [u,\bar{u},w]
16  i  ..2  x,x,0 [u,u,0]  \bar{x},x,0 [\bar{u},\bar{u},0]  x,x,0 [0,0,0]  x,x,0 [u,\bar{u},0]
\bar{x}+1/2,x+1/2,0 [u,u,0]  x+1/2,\bar{x}+1/2,0 [0,0,0]  x+1/2,\bar{x}+1/2,0 [u,\bar{u},0]  x+1/2,x+1/2,0 [u,u,0]
8  h  2.mm  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]
8  g  4..  0,0,z [0,0,w]  0,0,z [0,0,\bar{w}]  0,1/2,1/2 [0,0,0]  0,1/2,1/2 [0,0,\bar{w}]
8  f  .2/m'  1/4,1/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]
8  e  .2/m  1/4,1/4,0 [u,u,0]  3/4,3/4,0 [\bar{u},\bar{u},0]  3/4,1/4,0 [\bar{u},\bar{u},0]  1/4,3/4,0 [u,\bar{u},0]
4  d  \bar{4}2m  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]
4  c  \bar{4}2m  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]
4  b  42'2'  0,0,1/2 [0,0,w]  1/2,1,1/2 [0,0,0]
4  a  422  0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4mm1'  
\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2  \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2  
Origin at 0,0,z

Along [1,0,0]  p\text{mm}  
\mathbf{a}^* = \mathbf{b}/2  \quad \mathbf{b}^* = \mathbf{c}  
Origin at 1/4,1/2

Along [1,1,0]  p\text{2mm1'}  
\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2  \quad \mathbf{b}^* = \mathbf{c}  
Origin at x,x,0
P_2c 4'/nb'm
125.11.1041
P_2c 4'/n2'/b'2/m

4/mmm1'
Tetragonal

125.11.1041 - 1 - 2121
Origin at $4'2'2$ at $4'/n2'2/g$, at $-1/4,-1/4,0$ from center ($2/m$)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

Symmetry Operations

For $(0,0,0) +$ set

$(1) \quad 1$
$(1 | 0,0,0)$

$(2) \quad 2\quad 0,0,z$
$(2z | 0,0,0)$

$(3) \quad 4^*\quad 0,0,z$
$(4z | 0,0,0)'$

$(4) \quad 4^*\quad 0,0,z$
$(4z | 0,0,0)'$

$(5) \quad 2^*\quad 0,y,0$
$(2z | 0,0,0)'$

$(6) \quad 2'\quad x,0,0$
$(2z | 0,0,0)'$

$(7) \quad 2'\quad x,x,0$
$(2xy | 0,0,0)$

$(8) \quad 2\quad x,x,0$
$(2xy | 0,0,0)$

$(9) \quad \bar{T}^\perp\quad 1/4,1/4,0$
$(\bar{T} | 1/2,1/2,0)$

$(10) \quad n\quad (1/2,1/2,0)\quad x,y,0$
$(mz | 1/2,1/2,0)$

$(11) \quad 4^*\quad 1/2,0,z; 1/2,0,0$
$(4z | 1/2,1/2,0)'$

$(12) \quad 4^*\quad 0,1/2,z; 0,1/2,0$
$(4z | 1/2,1/2,0)'$

$(13) \quad a'(1/2,0,0)\quad x,1/4,z$
$(mz | 1/2,1/2,0)'$

$(14) \quad b'(0,1/2,0)\quad 1/4,y,z$
$(mz | 1/2,1/2,0)'$

$(15) \quad m\quad x+1/2,x,z$
$(mz | 1/2,1/2,0)$

$(16) \quad n\quad (1/2,1/2,1)\quad x,x,z$
$(mz | 1/2,1/2,1)$

For $(0,0,1) +$ set

$(1) \quad t'(0,0,1)$
$(1 | 0,0,1)'$

$(2) \quad 2'\quad (0,0,1)$
$(2z | 0,0,1)'$

$(3) \quad 4^*\quad (0,0,1)\quad 0,0,z$
$(4z | 0,0,1)$

$(4) \quad 4^*\quad (0,0,1)\quad 0,0,z$
$(4z | 0,0,1)$

$(5) \quad 2\quad 0,y,1/2$
$(2z | 0,0,1)$

$(6) \quad 2\quad x,0,1/2$
$(2z | 0,0,1)$

$(7) \quad 2'\quad x,x,1/2$
$(2xy | 0,0,1)'$

$(8) \quad 2'\quad x,x,1/2$
$(2xy | 0,0,1)'$

$(9) \quad \bar{T}^\perp\quad 1/4,1/4,1/2$
$(\bar{T} | 1/2,1/2,1)'$

$(10) \quad n'\quad (1/2,1/2,0)\quad x,y,1/2$
$(mz | 1/2,1/2,1)'$

$(11) \quad 4^*\quad 1/2,0,z; 1/2,0,1/2$
$(4z | 1/2,1/2,1)$

$(12) \quad 4^*\quad 0,1/2,z; 0,1/2,1/2$
$(4z | 1/2,1/2,1)$

$(13) \quad n\quad (1/2,0,1)\quad x,1/4,z$
$(mz | 1/2,1/2,1)$

$(14) \quad n\quad (0,1/2,1)\quad 1/4,y,z$
$(mz | 1/2,1/2,1)$

$(15) \quad c'(0,0,1)\quad x+1/2,x,z$
$(mz | 1/2,1/2,1)'$

$(16) \quad n'\quad (1/2,1/2,1)\quad x,x,z$
$(mz | 1/2,1/2,1)'$

Generators selected $(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9)$.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td>32</td>
<td>n</td>
<td>1</td>
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</table>

(1) $x,y,z\ [u,v,w]$

(2) $x,y,z\ [u,v,w]$

(3) $y,x,z\ [v,u,w]$

(4) $y,x,z\ [v,u,w]$

(5) $x,y,z\ [u,v,w]$

(6) $x,y,z\ [u,v,w]$

(7) $y,x,z\ [v,u,w]$

(8) $y,x,z\ [v,u,w]$

(9) $x+1/2,y+1/2,z\ [u,v,w]$

(10) $x+1/2,y+1/2,z\ [u,v,w]$

(11) $y+1/2,x+1/2,z\ [v,u,w]$

(12) $y+1/2,x+1/2,z\ [v,u,w]$

(13) $x+1/2,y+1/2,z\ [u,v,w]$

(14) $x+1/2,y+1/2,z\ [u,v,w]$

(15) $y+1/2,x+1/2,z\ [v,u,w]$

(16) $y+1/2,x+1/2,z\ [v,u,w]$
Symmetry of Special Projections

Along [0,0,1] \( p4mm1' \)
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] \( p_{2a}2m'm' \)
\[ a^* = -c \quad b^* = b/2 \]
Origin at x,0,1/2

Along [1,1,0] \( p2mm1' \)
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,0
$P_2c\ 4'/nmb'$

$4/mmm1'$

Tetragonal

125.12.1042

$P_2c\ 4'/n2/b2'/m'$
Origin at 4'22' at 4'/n22'/g', at -1/4,-1/4,0 from center (2'/m')

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1  (2) 2  0,0,z
(1) | 0,0,0  (2) z | 0,0,0
(5) 2  0,y,0  (6) 2  x,0,0
(5) y | 0,0,0  (6) z | 0,0,0
(9) T' 1/4,1/4,0  (10) n' (1/2,1/2,0)  x,y,0
(9) z | 1/2,1/2,0  (10) z | 1/2,1/2,0
(13) a (1/2,0,0)  x,1/4,z  (14) b (0,1/2,0)  1/4,y,z
(13) 1/2,1/2,0  (14) 1/2,1/2,0

For (0,0,1)' + set

(1) t' (0,0,1)  (2) 2'  0,0,z
(1) | 0,0,1  (2) z | 0,0,1
(5) 2'  0,y,1/2  (6) 2'  x,0,1/2
(5) y | 0,0,1  (6) z | 0,0,1
(9) T' 1/4,1/4,1/2  (10) n' (1/2,1/2,0)  x,y,1/2
(9) z | 1/2,1/2,1  (10) z | 1/2,1/2,1
(13) a (1/2,0,1)  x,1/4,z  (14) b (0,1/2,1)  1/4,y,z
(13) 1/2,1/2,1  (14) 1/2,1/2,1

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<td>(0,0,1)' +</td>
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<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
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</tr>
<tr>
<td>(13) x+1/2,y+1/2,z [u,v,w]</td>
<td>(14) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>16</td>
<td>m'</td>
</tr>
<tr>
<td>x,x+1/2,z [u,u,w]</td>
<td>x,x+1/2,z [u,u,w]</td>
</tr>
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<td>x,x+1/2,z [u,u,w]</td>
<td>x,x+1/2,z [u,u,w]</td>
</tr>
</tbody>
</table>
16  l .2'.  x,0,1/2 [0,v,w]    x,0,1/2 [0,v,w]    0,x,1/2 [v,0,w]    0,x,1/2 [v,0,w]  
   x+1/2,1/2,1/2 [0,v,w] x+1/2,1/2,1/2 [0,v,w] 1/2,x+1/2,1/2 [v,0,w] 1/2,x+1/2,1/2 [v,0,w]  
16  k .2.  x,0,0 [u,0,0]    x,0,0 [u,0,0]    0,x,0 [0,u,0]    0,x,0 [0,u,0]  
   x+1/2,1/2,0 [u,0,0] x+1/2,1/2,0 [u,0,0] 1/2,x+1/2,0 [u,0,0] 1/2,x+1/2,0 [u,0,0]  
16  j .2  x,x,1/2 [u,u,0] x,x,1/2 [u,u,0]    x,x,1/2 [u,u,0]    x,x,1/2 [u,u,0]  
   x+1/2,x+1/2,1/2 [u,u,0] x+1/2,x+1/2,1/2 [u,u,0] 1/2,x+1/2,x [u,u,0] 1/2,x+1/2,x [u,u,0]  
16  i .2'  x,x,0 [u,u,w]    x,x,0 [u,u,w]    x,x,0 [u,u,w]    x,x,0 [u,u,w]  
   x,x,0 [u,u,w]    x,x,0 [u,u,w]    x,x,0 [u,u,w]    x,x,0 [u,u,w]  
   x+1/2,x+1/2,2 [u,u,w] x+1/2,x+1/2,2 [u,u,w] 1/2,x+1/2,x [u,u,w] 1/2,x+1/2,x [u,u,w]  
8   h 2.m'm'  0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 0,1/2,z [0,0,w] 1/2,0,z [0,0,w]  
8   g 4'.  0,0,2 [0,0,0]    0,0,2 [0,0,0]    1/2,1/2,2 [0,0,0]    1/2,1/2,2 [0,0,0]  
8   f .2/m'  1/4,1/4,1/2 [0,0,0] 3/4,3/4,1/2 [0,0,0] 3/4,1/4,1/2 [0,0,0] 1/4,3/4,1/2 [0,0,0]  
8   e .2'/m' 1/4,1/4,0 [u,u,w] 3/4,3/4,0 [u,u,w] 3/4,1/4,0 [u,u,w] 1/4,3/4,0 [u,u,w]  
4   d 42'2m'  0,1/2,1/2 [0,0,w] 1/2,0,1/2 [0,0,w]  
4   c 42'2m'  0,1/2,0 [0,0,0]    0,1/2,0 [0,0,0]  
4   b 4'2'2  0,0,1/2 [0,0,0]    1/2,1/2,1/2 [0,0,0]  
4   a 4'2'2'  0,0,0 [0,0,0]    1/2,1/2,0 [0,0,0]  

Symmetry of Special Projections  
Along [0,0,1] p4mm1'  Along [1,0,0] p2mm  Along [1,1,0] p222m'  
\( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  \( a^* = b/2 \)  \( b^* = c \)  \( a^* = -c \)  \( b^* = (-a + b)/2 \)  
Origin at 0,0,z  Origin at x,1/4,1/2  Origin at x,x,1/2
$P_{2c} 4/\text{nb}'m'$

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$4/\text{mmm}1'$

Tetragonal

$P_{2c} 4/n2'/b'2'/m'$
Origin at 42'2' at 4/n2'2'/g', at -1/4,-1/4,0 from center (2'/m')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x \]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(5) & \quad 1/4,1/4,0 \\
(13) & \quad 1/2,0,0 \\
(1) & \quad t(0,0,1) \\
(1) & \quad 0,0,1 \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
(1) & \quad t'(0,0,1) \\
(1) & \quad 0,0,1' \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
(1) & \quad t(0,0,1) \\
(1) & \quad 0,0,1 \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
(1) & \quad t'(0,0,1) \\
(1) & \quad 0,0,1' \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
(1) & \quad t(0,0,1) \\
(1) & \quad 0,0,1 \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
(1) & \quad t'(0,0,1) \\
(1) & \quad 0,0,1' \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
\end{align*}
\]

for \((0,0,1)\)' + set

\[
\begin{align*}
(1) & \quad t'(0,0,1) \\
(1) & \quad 0,0,1' \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
(1) & \quad t(0,0,1) \\
(1) & \quad 0,0,1 \\
(5) & \quad 0,y,1/2 \\
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(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
(1) & \quad t(0,0,1) \\
(1) & \quad 0,0,1 \\
(5) & \quad 0,y,1/2 \\
(9) & \quad -1/4,1/4,1/2 \\
(13) & \quad 1/2,0,1 \\
\end{align*}
\]

Generators selected

\[(1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (9).\]

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

\[
\begin{align*}
&32 \quad n \quad 1 \\
&\begin{align*}
(1) & \quad x,y,z \quad [u,v,w] \\
(5) & \quad x,y,z \quad [u,v,w] \\
(9) & \quad x+1/2,y+1/2,z \quad [u,v,w] \\
(13) & \quad x+1/2,y+1/2,z \quad [u,v,w] \\
16 & \quad m \quad ..m' \\
\end{align*}
\end{align*}
\]

Coordinates

\[
\begin{align*}
(0,0,0) & \quad + \quad (0,0,1) \\
(0,0,0) & \quad + \quad (0,0,1) \\
\end{align*}
\]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Special Projections</th>
<th>Along [0,0,1]</th>
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<tbody>
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<td>p4mm1'</td>
<td>p\text{22} m'</td>
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</tr>
<tr>
<td>a* = (a - b)/2</td>
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<td></td>
</tr>
</tbody>
</table>
Origin at 422/n, at -1/4,-1/4,-1/4 from \( \bar{1} \)

Asymmetric unit: \( 0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/4 \)

Symmetry Operations:

1. \( 1 \)
   \( (1) \ 0,0,0 \)

2. \( 0,y,0 \)
   \( (2) \ x,0,0 \)

3. \( 0,0,0 \)
   \( (3) \ 4^+ \ x,0,0 \)

4. \( 0,0,0 \)
   \( (4) \ 4^- \ 0,0,0 \)

5. \( 0,y,0 \)
   \( (5) \ 2^0 \ x,0,0 \)

6. \( 0,y,0 \)
   \( (6) \ 2^0 \ 0,0,0 \)

7. \( 0,y,0 \)
   \( (7) \ 2^0 \ x,0,0 \)

8. \( 0,y,0 \)
   \( (8) \ 2^0 \ 0,0,0 \)

9. \( 1/4,1/4,1/4 \)
   \( (9) \ -1/2,1/2,1/2 \)

10. \( x,y,1/4 \)
    \( (10) \ 1/2,1/2,0 \)

11. \( 4^+ \ x,0,0 \)
    \( (11) \ 4^- \ 0,1/2,z \)

12. \( 4^+ \ x,0,0 \)
    \( (12) \ 4^- \ 0,1/2,z \)

13. \( x,1/4,z \)
    \( (13) \ 1/2,0,1/2 \)

14. \( 1/4,y,z \)
    \( (14) \ 0,1/2,1/2 \)

15. \( x,1/4,z \)
    \( (15) \ 0,0,1/2 \)

16. \( x,1/4,z \)
    \( (16) \ 0,0,1/2 \)

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### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
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<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
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<tr>
<td>8</td>
<td>j .2</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x+1/2,1/2,0 [u,0,0]</td>
<td>1/2,x+1/2,0 [0,u,0]</td>
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<td>0,x,1/2 [0,u,0]</td>
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<td>8</td>
<td>h .2</td>
<td>x,x,0 [u,u,0]</td>
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<td>x+1/2,x+1/2,1/2 [u,u,0]</td>
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<td>1/2,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
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<td></td>
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<td>1/2,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>e 4</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<td>1/2,0,3/4 [0,0,w]</td>
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<td>4</td>
<td>c 222.</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
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<td>2</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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<td>2</td>
<td>a 422</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] \ p_p, 4m'\m'
\[ a^* = (a \ - \ b)/2 \quad b^* = (a \ + \ b)/2 \]
Origin at 0,0,z

Along [1,0,0] \ c_p, 2m'\m'
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] \ p_{2a}, 2m'\m'
\[ a^* = -c/2 \quad b^* = (-a + b)/2 \]
Origin at x,x,0
Origin at $422/n1'$, at -1/4,-1/4,-1/4 from $1'$.  

Asymmetric unit:

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $1+$ set:

1. $1 \quad (0,0,0)$
2. $2 \quad 0,0,z \quad (2z,0,0,0)$
3. $4' \quad 0,0,z \quad (4z,0,0,0)$
4. $4' \quad 0,0,z \quad (4z,0,0,0)$
5. $2 \quad y,0 \quad (2y,0,0,0)$
6. $2 \quad x,0 \quad (2x,0,0,0)$
7. $2 \quad x,x,0 \quad (2x,0,0,0)$
8. $2 \quad x,x,0 \quad (2x,0,0,0)$
9. $\bar{2} \quad 1/4,1,1/4 \quad (0,1/2,1/2)$
10. $n \quad (1/2,1/2,0) \quad x,y,1/4 \quad (m_{y},1/2,1/2,1/2)$
11. $\bar{4} \quad 1/2,0,z ; 1/2,0,1/4 \quad (4z,1/2,1/2,1/2)$
12. $\bar{4} \quad 0,1/2,z ; 0,1/2,1/4 \quad (4z,1/2,1/2,1/2)$
13. $n \quad (1/2,0,1/2) \quad x,1/4,z \quad (m_{y},1/2,1/2,1/2)$
14. $n \quad (0,1/2,1/2) \quad 1/4,y,z \quad (m_{y},1/2,1/2,1/2)$
15. $c \quad (0,0,1/2) \quad x+1/2,x,z \quad (m_{y},1/2,1/2,1/2)$
16. $n \quad (1/2,1/2,1/2) \quad x,x,z \quad (m_{y},1/2,1/2,1/2)$
Continued

For 1′ + set

(1) 1′
   (1) (0,0,0)′

(2) 2′ 0,0,z
   (2) (0,0,0)′

(3) 4+′ 0,0,z
   (4) (0,0,0)′

(4) 4′ - 0,0,z
   (4) (0,0,0)′

(5) 0,y,0
   (2) (0,0,0)′

(6) 2′ x,0,0
   (2) (0,0,0)′

(7) 2′ x,x,0
   (2) (0,0,0)′

(8) 2′ x,x,0
   (2) (0,0,0)′

(9) 1′ 1/4,1/4,1/4
   (2) 1/2,1/2,1/2)

(10) n′ (1/2,1/2,1/2) x,y,1/4
    (m) 1/2,1/2,1/2)

(11) n′ (1/2,1/2,1/2) x+1/2,x+1/2,1/2 [0,0,0]
    (m) 1/2,1/2,1/2)

(12) n′ (1/2,1/2,1/2) x,x,z
    (1/2,1/2,1/2)

(13) n′ (1/2,1/2,1/2) x,1/4,z
    (m) 1/2,1/2,1/2)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1′.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

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<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<th>Coordinates</th>
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<td>1′ +</td>
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### Symmetry of Special Projections

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<tr>
<td>4 e</td>
<td>4..1'</td>
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<td>0,0,\overline{z} [0,0,0]</td>
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<td>1/2,1/2,\overline{z}+1/2 [0,0,0]</td>
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<td>\overline{4}..1'</td>
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<td>222.1'</td>
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### Origin

- **Along [0,0,1]**: p 4mm1'
  - \(a^* = (a - b)/2\)
  - \(b^* = (a + b)/2\)
  - Origin at 0,0,z

- **Along [1,0,0]**: c 2mm1'
  - \(a^* = b\)
  - \(b^* = c\)
  - Origin at x,0,0

- **Along [1,1,0]**: p 2mm1'
  - \(a^* = (-a + b)/2\)
  - \(b^* = c/2\)
  - Origin at x,x,0
### Origin
At 42'2'/n, at -1/4,-1/4,-1/4 from 1

### Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

### Symmetry Operations

1. 1
   
2. $2\cdot 0,0,z$
   
3. $4^+\cdot 0,0,z$
   
4. $4^-\cdot 0,0,z$

5. $2'\cdot 0,y,0$

6. $2'\cdot x,0,0$

7. $2'\cdot x,x,0$

8. $2'\cdot x,x,0$

9. $\overline{1}\cdot 1/4,1/4,1/4$

10. $n'\cdot (1/2,1/2,0)$

11. $\overline{4}^-\cdot 1/2,0,0$

12. $\overline{4}^-\cdot 0,1/2,0; 0,1/2,1/4$

13. $n\cdot (1/2,0,1/2)$

14. $n\cdot (0,1/2,1/2)$

15. $c\cdot (0,0,1/2)$

16. $n\cdot (1/2,1/2,1/2)$

17. $n\cdot (1/2,1/2,1/2)$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>.2'</td>
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<tr>
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<td>i</td>
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<td>8</td>
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#### Coordinates

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<td>(16)</td>
<td>y+1/2,x+1/2,z+1/2 [v,w]</td>
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Symmetry of Special Projections

Along [0,0,1] \( p \) 4mm
\( a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \)
Origin at 0,0,z

Along [1,0,0] \( c \) 2mm'
\( a^* = -c \quad b^* = b \)
Origin at x,0,0

Along [1,1,0] \( p_{2a'} \) 2m'm'
\( a^* = \frac{-c}{2} \quad b^* = \frac{-(a + b)}{2} \)
Origin at x,x,0
P4'/nn'c
126.4.1047

4'/mm'm
P4'/n2'/n'2/c

Tetragonal

**Origin** at 4'2'2/n, at -1/4,-1/4,-1/4 from \( \bar{1} \)

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

\begin{align*}
(1) & \ 1 \quad (1|0,0,0) \\
(2) & \ 2_x \ 0,0,z \quad (2_z|0,0,0) \\
(3) & \ 4''_x \ 0,0,z \quad (4_z|0,0,0)' \\
(4) & \ 4''_x \ 0,0,z \quad (4_z|-1,0,0)' \\
(5) & \ 2' \ 0,y,0 \quad (2_y|0,0,0)' \\
(6) & \ 2' \ x,0,0 \quad (2_x|0,0,0)' \\
(7) & \ 2 \ x,x,0 \quad (2_{xx}|0,0,0) \\
(8) & \ 2 \ x,x,0 \quad (2_{xx}|0,0,0) \\
(9) & \ \bar{1} \ 1/4,1/4,1/4 \quad (\bar{1}|1/2,1/2,1/2) \\
(10) & \ n \ (1/2,1/2,0) \quad x,y,1/4 \quad (m_x|1/2,1/2,1/2) \\
(11) & \ \bar{4}''_x \ 1/2,0,z \quad 1/2,0,1/4 \quad (\bar{4}_z|1/2,1/2,1/2)' \\
(12) & \ \bar{4}''_x \ 0,1/2,z \quad 0,1/2,1/4 \quad (\bar{4}_z|-1,1/2,1/2)' \\
(13) & \ n' \ (1/2,0,1/2) \quad x,1/4,z \quad (m_y|1/2,1/2,1/2)' \\
(14) & \ n' \ (0,1/2,1/2) \quad 1/4,y,z \quad (m_y|1/2,1/2,1/2)' \\
(15) & \ c \ (0,0,1/2) \quad x+1/2,x,z \quad (m_{xy}|1/2,1/2,1/2) \\
(16) & \ n \ (1/2,1/2,1/2) \quad x,x,z \quad (m_{xy}|1/2,1/2,1/2)
\end{align*}
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<th>Multiplicity</th>
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<td>(1) x,y,z [u,v,w]</td>
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<td>(3) y,x,z</td>
<td>[v,u,w]</td>
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<td>(5) x,y,z</td>
<td>[u,v,w]</td>
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<td>(7) y,x,z</td>
<td>[v,u,w]</td>
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<td>(9) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(10) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
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Continued 126.4.1047 P4'\text{inn}'c
Symmetry of Special Projections

Along [0,0,1] \( p \), 4mm
\( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)
Origin at 1/2,0,z

Along [1,0,0] \( c \), 2mm'
\( a^* = -c \) \( b^* = b \)
Origin at x,0,0

Along [1,1,0] \( p_{2a} \), 2m'm'
\( a^* = -c/2 \) \( b^* = (-a + b)/2 \)
Origin at x,x,0
**Origin** at 4'22'/n', at -1/4,-1/4,-1/4 from 1

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

1. **I**
   - (1) 1
     - (1 | 0,0,0)

2. **2**
   - (5) 2 0,y,0
     - (2z | 0,0,0)
   - (6) 2 x,0,0
     - (2z | 0,0,0)

3. **4'**
   - (10) n (1/2,1/2,0)
     - x,y,1/4
     - (m_\perp | 1/2,1/2,1/2)
   - (11) 4' * 1/2,0,z; 1/2,0,1/4
     - (4_{z} | 1/2,1/2,1/2)'

4. **4'**
   - (13) n (1/2,0,1/2)
     - x,1/4,z
     - (m_\perp | 1/2,1/2,1/2)
   - (14) n (0,1/2,1/2) 1/4,y,z
     - (m_\perp | 1/2,1/2,1/2)
   - (15) c' (0,0,1/2) x+1/2,x,z
     - (m_{xy} | 1/2,1/2,1/2)'

5. **n**
   - (12) n' (1/2,1/2,1/2) x,x,z
     - (m_{xy} | 1/2,1/2,1/2)'

6. **m**
   - (16) m' (1/2,1/2,1/2) x,x,z
     - (m_{xy} | 1/2,1/2,1/2)'

**Tetragonal**

\[ 126.5.1048 \]

**P4'/nnc'**

\[ 126.5.1048 \]

**P4'/mmm'**

\[ 126.5.1048 \]

**P4'/n2/n2'/c'**

\[ 126.5.1048 \]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

16  k  1  
(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) y,x,z [v,u,w]
(4) y,x,z [v,u,w]
(5) x,y,z [u,v,w]
(6) y,x,z [v,u,w]
(7) y,x,z [v,u,w]
(8) y+1/2,x+1/2,z+1/2 [u,v,w]
(9) x+1/2,y+1/2,z+1/2 [u,v,w]
(10) x+1/2,y+1/2,z+1/2 [u,v,w]

8  j  .2. 
(1) x,0,1/2 [u,0,0]
(2) x,0,1/2 [u,0,0]
(3) x+1/2,1/2,0 [u,0,0]
(4) x+1/2,1/2,0 [u,0,0]
(5) 0,x,1/2 [0,u,0]
(6) 0,x,1/2 [0,u,0]
(7) 0,x,1/2 [0,u,0]
(8) 0,x,1/2 [0,u,0]

8  i  .2. 
(1) x,0,0 [u,0,0]
(2) x,0,0 [u,0,0]
(3) x+1/2,1/2,1/2 [u,0,0]
(4) x+1/2,1/2,1/2 [u,0,0]
(5) 0,x,0 [0,u,0]
(6) 0,x,0 [0,u,0]
(7) 0,x,0 [0,u,0]
(8) 0,x,0 [0,u,0]

8  h  ..2' 
(1) x,x,0 [u,u,w]
(2) x,x,0 [u,u,w]
(3) x,x,0 [u,u,w]
(4) x,x,0 [u,u,w]

8  g  2.. 
(1) 1/2,0,z [0,0,w]
(2) 1/2,0,z [0,0,w]
(3) 1/2,0,z [0,0,w]
(4) 1/2,0,z [0,0,w]

8  f  1' 
(1) 1/4,1,4/4 [u,v,w]
(2) 1/4,1,4/4 [u,v,w]
(3) 1/4,1,4/4 [u,v,w]
(4) 1/4,1,4/4 [u,v,w]

4  e  4'.. 
(1) 0,0,z [0,0,0]
(2) 0,0,z [0,0,0]
(3) 0,0,z [0,0,0]
(4) 0,0,z [0,0,0]

4  d  4'.. 
(1) 0,1/2,1/2 [0,1/2,1/2]
(2) 0,1/2,1/2 [0,1/2,1/2]
(3) 0,1/2,1/2 [0,1/2,1/2]
(4) 0,1/2,1/2 [0,1/2,1/2]

4  c  222. 
(1) 1/2,0,0 [0,0,0]
(2) 1/2,0,0 [0,0,0]
(3) 1/2,0,0 [0,0,0]
(4) 1/2,0,0 [0,0,0]

2  b  4'22' 
(1) 0,0,0 [0,0,0]
(2) 0,0,0 [0,0,0]

2  a  4'22' 
(1) 0,0,0 [0,0,0]
(2) 0,0,0 [0,0,0]
Symmetry of Special Projections

Along [0,0,1] \( p' \), \( 4m'm' \)
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at \( 1/2,0,z \)

Along [0,0,0] \( c \), \( 2m'm' \)
\[ a^* = b \quad b^* = c \]
Origin at \( x,0,0 \)

Along [1,1,0] \( p \), \( 2'm'm' \)
\[ a^* = -c/2 \quad b^* = (-a + b)/2 \]
Origin at \( x,x,0 \)
Origin at $4'22'/n'$, at -1/4,-1/4,-1/4 from $\bar{1}'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $1 \quad (1 | 0,0,0)$
2. $2 \quad 0,0,z \quad (2_z | 0,0,0)$
3. $4' \quad 0,0,z \quad (4_z | 0,0,0)'$
4. $4' \quad 0,0,z \quad (4_z | 0,0,0)'$
5. $2 \quad 0,y,0 \quad (2_z | 0,0,0)$
6. $2 \quad x,0,0 \quad (2_x | 0,0,0)$
7. $2' \quad x,x,0 \quad (2_{xy} | 0,0,0)'$
8. $2' \quad x,x,0 \quad (2_{xy} | 0,0,0)'$
9. $1/4,1/4,1/4 \quad (1 | 1/2,1/2,1/2)'$
10. $n' \quad 1/2,1/2,0 \quad x,y,1/4 \quad (m_1 | 1/2,1/2,1/2)'$
11. $4' \quad 1/2,0,z; 1/2,0,1/4 \quad (4_z | 1/2,1/2,1/2)$
12. $4' \quad 1/2,0,z; 1/2,0,1/4 \quad (4_z | 1/2,1/2,1/2)$
13. $n' \quad 1/2,0,1/2 \quad x,1/4,z \quad (m_1 | 1/2,1/2,1/2)'$
14. $n' \quad 0,1/2,1/2 \quad 1/4,y,z \quad (m_1 | 1/2,1/2,1/2)'$
15. $c \quad (0,0,1/2) \quad x+1/2,x,z \quad (m_1 | 1/2,1/2,1/2)$
16. $n \quad 1/2,1/2,1/2 \quad x,x,z \quad (m_1 | 1/2,1/2,1/2)$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>k 1</td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(2) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(3) y,x,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(4) y,x,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(5) x,y,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(6) x,y,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(7) y,x,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(8) x+1/2,y+1/2,z+1/2</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(9) y+1/2,x+1/2,z+1/2</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(10) x+1/2,y+1/2,z+1/2</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(11) y+1/2,x+1/2,z+1/2</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(12) x+1/2,y+1/2,z+1/2</td>
<td>[u,v,w]</td>
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<tr>
<td>(13) y+1/2,x+1/2,z+1/2</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(14) x+1/2,y+1/2,z+1/2</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(15) y+1/2,x+1/2,z+1/2</td>
<td>[v,u,w]</td>
</tr>
</tbody>
</table>

| 8 j .2.      | x,0,1/2 [u,0,0] |
| 8 i .2.      | x,0,0 [u,0,0] |
| 8 h .2'      | x,x,0 [u,u,w] |
| 8 g 2..      | 1/2,0,z [0,0,0] |
| 8 f 4'..     | 1/4,1/4,1/4 [0,0,0] |
| 4 e 4'..     | 0,0,z [0,0,0] |
| 4 d 4'..     | 1/2,0,1/4 [0,0,0] |
| 4 c 222.     | 1/2,0,0 [0,0,0] |

Continued

126.6.1049 - 2 - 2146
Symmetry of Special Projections

Along [0,0,1]  p4'mm'  
\[ a^* = \frac{a - b}{2} \quad b^* = \frac{a + b}{2} \]
Origin at 0,0,z

Along [1,0,0]  c 2m'm'  
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0]  p 2a* 2mm  
\[ a^* = -\frac{c}{2} \quad b^* = \frac{-a + b}{2} \]
Origin at x-1/4,x+1/4,0
Origin at 42'2'/n', at -1/4,-1/4,-1/4 from 1

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1 (1|0,0,0)
(5) 2' 0,y,0
(2) 2 0,0,z
(2_2|0,0,0)
(3) 4+ 0,0,z
(4_2|0,0,0)
(4) 4' 0,0,z
(4_2|0,0,0)
(2y|0,0,0)
(2 x|0,0,0)
(2 xy|0,0,0)
(2 x|y|0,0,0)

(9) 1/4,1/4,1/4
(1/2,1/2,1/2)
(10) n (1/2,1/2,0) x,y,1/4
(m_2|1/2,1/2,1/2)
(11) 4+ 1/2,0,z; 1/2,0,1/4
(4_2|1/2,1/2,1/2)
(12) 4' 0,1/2,z; 0,1/2,1/4
(4_2|1/2,1/2,1/2)
(13) n' (1/2,0,1/2) x,1/4,z
(m_2|1/2,1/2,1/2)
(14) n' (0,1/2,1/2) 1/4,y,z
(m_2|1/2,1/2,1/2)
(15) c' (0,0,1/2) x+1/2,x,z
(m_2|1/2,1/2,1/2)
(16) n' (1/2,1/2,1/2) x,x,z
(m_2|1/2,1/2,1/2)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>16</td>
<td>k</td>
<td>1</td>
</tr>
<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
<td>(2) x, y, z  [u, v, w]</td>
</tr>
<tr>
<td>(3)</td>
<td>y,x,z [v,u,w]</td>
<td>(4) y, x, z  [v, u, w]</td>
</tr>
<tr>
<td>(5)</td>
<td>x,y,z [u,v,w]</td>
<td>(6) x, y, z  [u, v, w]</td>
</tr>
<tr>
<td>(7)</td>
<td>y,x,z [v,u,w]</td>
<td>(8) y, x, z  [v, u, w]</td>
</tr>
<tr>
<td>(9)</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(10) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td>(11)</td>
<td>y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(12) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<tr>
<td>(13)</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(14) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(15)</td>
<td>y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>j</td>
<td>.2'</td>
</tr>
<tr>
<td>(2)</td>
<td>x,0,1/2 [0,v,w]</td>
<td>x,0,1/2 [0,v,w]</td>
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<tr>
<td>(3)</td>
<td>x+1/2,1/2,0 [0,v,w]</td>
<td>x+1/2,1/2,0 [0,v,w]</td>
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<tr>
<td>(4)</td>
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<td>(5)</td>
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<td>x+1/2,1/2,1/2 [0,v,w]</td>
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<td>(6)</td>
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<td>(7)</td>
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<td>x+1/2,x+1/2,1/2 [u,u,w]</td>
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<td>(8)</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
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<td>(9)</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
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<tr>
<td>(10)</td>
<td>1/4,3/4,1/4 [u,v,w]</td>
<td>1/4,3/4,1/4 [u,v,w]</td>
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<tr>
<td>(11)</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<td>(12)</td>
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<td>1/2,1/2,z+1/2 [0,0,0]</td>
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<td>(13)</td>
<td>1/2,0,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
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<td>(14)</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
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<tr>
<td>(15)</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<tr>
<td>(16)</td>
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<td>0,0,0 [0,0,0]</td>
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### Coordinates

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>16 k 16</td>
<td>x, y, z [u, v, w]</td>
</tr>
<tr>
<td>3 (1)</td>
<td>y, x, z [v, u, w]</td>
</tr>
<tr>
<td>5 (2)</td>
<td>x, y, z [u, v, w]</td>
</tr>
<tr>
<td>6 (3)</td>
<td>y, x, z [v, u, w]</td>
</tr>
<tr>
<td>9 (4)</td>
<td>y + 1/2, y + 1/2, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td>11 (5)</td>
<td>y + 1/2, x + 1/2, z + 1/2 [v, u, w]</td>
</tr>
<tr>
<td>13 (6)</td>
<td>x + 1/2, y + 1/2, z + 1/2 [u, v, w]</td>
</tr>
<tr>
<td>15 (7)</td>
<td>y + 1/2, x + 1/2, z + 1/2 [v, u, w]</td>
</tr>
<tr>
<td>8 j 8</td>
<td>x, 0, 1/2 [0, v, w]</td>
</tr>
<tr>
<td>9 (8)</td>
<td>x + 1/2, 1/2, 0 [0, v, w]</td>
</tr>
<tr>
<td>11 (9)</td>
<td>x, 0, 0 [0, v, w]</td>
</tr>
<tr>
<td>13 (10)</td>
<td>x + 1/2, 1/2, 1/2 [0, v, w]</td>
</tr>
<tr>
<td>15 (11)</td>
<td>x + 1/2, x + 1/2, 1/2 [u, u, w]</td>
</tr>
<tr>
<td>8 i 8</td>
<td>x, x, 0 [u, u, w]</td>
</tr>
<tr>
<td>9 (12)</td>
<td>x + 1/2, x + 1/2, 1/2 [u, u, w]</td>
</tr>
<tr>
<td>11 (13)</td>
<td>1/2, 0, z [0, 0, w]</td>
</tr>
<tr>
<td>13 (14)</td>
<td>1/2, 0, z + 1/2 [0, 0, w]</td>
</tr>
<tr>
<td>15 (15)</td>
<td>1/4, 3/4, 1/4 [u, v, w]</td>
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<td>17 (16)</td>
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<td>19 (17)</td>
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<td>20 (18)</td>
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<td>21 (19)</td>
<td>0, 1/2, 1/4 [0, 0, 0]</td>
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<tr>
<td>25 (23)</td>
<td>1/2, 1/2, 1/2 [0, 0, 0]</td>
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**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Formula</th>
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</thead>
<tbody>
<tr>
<td>Along $[0,0,1]$</td>
<td>$p_{14}$ 4mm</td>
<td>$a^* = (a - b)/2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = (a + b)/2$</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along $[1,0,0]$</td>
<td>$c_{2}'mm'$</td>
<td>$a^* = -c$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b$</td>
</tr>
<tr>
<td>Origin at $x,0,0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along $[1,1,0]$</td>
<td>$p_{2m}'m'$</td>
<td>$a^* = (-a + b)/2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = c/2$</td>
</tr>
<tr>
<td>Origin at $x,x,0$</td>
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<td></td>
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</tbody>
</table>
Origin at 422/n’, at -1/4,-1/4,-1/4 from 1

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2z 0,0,z
(2z | 0,0,0)

(3) 4h 0,0,z
(4z | 0,0,0)

(4) 4h 0,0,z
(4z | 0,0,0)

(5) 2t 0,y,0
(2y | 0,0,0)

(6) 2h x,0,0
(2s | 0,0,0)

(7) 2h x,x,0
(2xy | 0,0,0)

(8) 2h x,x,0
(2xy | 0,0,0)

(9) 2h 1/4,1/4,1/4
(2h | 1/2,1/2,1/2)

(10) n’ (1/2,1/2,0) x,y,1/4
(m | 1/2,1/2,1/2)

(11) 4h 1/2,0,z; 1/2,0,1/4
(4z | 1/2,1/2,1/2)

(12) 4h 0,1/2,z; 0,1/2,1/4
(4z | 1/2,1/2,1/2)

(13) n’ (1/2,0,1/2) x,1/4,z
(m | 1/2,1/2,1/2)

(14) n (0,1/2,1/2) 1/4,y,z
(m | 1/2,1/2,1/2)

(15) c’ (0,0,1/2) x+1/2,x,z
(mxy | 1/2,1/2,1/2)

(16) n’ (1/2,1/2,1/2) x,x,z
(mxy | 1/2,1/2,1/2)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<td>k</td>
<td>1</td>
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#### Coordinates

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<tr>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
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<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(9) x+y/2,y+z/2,z+1/2 [u,v,w]</td>
<td>(10) x+y/2,y+z/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(11) y+x/2,z+y/2,z+1/2 [v,u,w]</td>
<td>(12) y+x/2,z+y/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(13) x+y/2,y+z/2,z+1/2 [u,v,w]</td>
<td>(14) x+y/2,y+z/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(15) y+x/2,x+y/2,z+1/2 [v,u,w]</td>
<td>(16) y+x/2,x+y/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

#### Additional coordinates

| 8 | j | .2' | x,0,1/2 [0,v,w] |
| 8 | i | .2' | x,0,0 [0,v,w] |
| 8 | h | .2 | x,x,0 [u,u,0] |

| 8 | g | 2' | 1/2,0,z [0,0,w] |
| 8 | f | 1' | 1/4,1/4,1/4 [0,0,0] |
| 4 | e | 4' | 0,0,0 [0,0,0] |
| 4 | d | 4' | 1/2,0,1/4 [0,0,w] |
| 4 | c | 22'2' | 1/2,0,0 [0,0,w] |
| 2 | b | 42'2 | 0,0,1/2 [0,0,0] |
| 2 | a | 42'2 | 0,0,0 [0,0,0] |
Symmetry of Special Projections

Along [0,0,1] $p' 4'm'm$
\begin{align*}
a^* &= \frac{(a - b)}{2} \\
b^* &= \frac{(a + b)}{2}
\end{align*}
Origin at 0,0,z

Along [1,0,0] $c'$ $2'mm'$
\begin{align*}
a^* &= -c \\
b^* &= b
\end{align*}
Origin at x,0,0

Along [1,1,0] $p 2m'm'$
\begin{align*}
a^* &= \frac{(-a + b)}{2} \\
b^* &= \frac{c}{2}
\end{align*}
Origin at x,x,0
P4/n'c'
126.9.1052

4/m'm'm'
P4/n'2/n'2/c'

Tetragonal

Origin at 422/n', at -1/4,-1/4,-1/4 from 1

Asymmetric unit 0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4

Symmetry Operations

1. 1
   (1 | 0,0,0)

2. 2 0,0,z
   (2_z | 0,0,0)

3. 4+ 0,0,z
   (4_z | 0,0,0)

4. 4- 0,0,z
   (4_z^{-1} | 0,0,0)

5. 2 0,y,0
   (2_y | 0,0,0)

6. 2 x,0,0
   (2_x | 0,0,0)

7. 2 x,x,0
   (2_{xy} | 0,0,0)

8. 2 x,x,0
   (2_{xy} | 0,0,0)

9. 1' 1/4,1/4,1/4
   (1' | 1/2,1/2,1/2)'

10. n' (1/2,1/2,0) x,y,1/4
    (m_x | 1/2,1/2,1/2)'

11. 4+ 1/2,0,z; 1/2,0,1/4
    (4_z | 1/2,1/2,1/2)'

12. 4+ 1/2,0,z; 0,1/2,1/4
    (4_z^{-1} | 1/2,1/2,1/2)'

13. n' (1/2,0,1/2) x,1/4,z
    (m_y | 1/2,1/2,1/2)'

14. n' (0,1/2,1/2) 1/4,y,z
    (m_y | 1/2,1/2,1/2)'

15. c' (0,0,1/2) x+1/2,x,z
    (m_{xy} | 1/2,1/2,1/2)'

16. n' (1/2,1/2,1/2) x,x,z
    (m_{xy} | 1/2,1/2,1/2)'

126.9.1052 - 1 - 2154
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

16 k 1
(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) y,x,z [v,u,w]
(4) y,x,z [v,u,w]
(5) x,y,z [u,v,w]
(6) x,y,z [u,v,w]
(7) y,x,z [v,u,w]
(8) y,x,z [v,u,w]
(9) x+1/2,y+1/2,z+1/2 [u,v,w]
(10) x+1/2,y+1/2,z+1/2 [u,v,w]
(11) y+1/2,x+1/2,z+1/2 [v,u,w]
(12) y+1/2,x+1/2,z+1/2 [v,u,w]
(13) x+1/2,y+1/2,z+1/2 [u,v,w]
(14) x+1/2,y+1/2,z+1/2 [u,v,w]
(15) x+1/2,y+1/2,z+1/2 [v,u,w]
(16) y+1/2,x+1/2,z+1/2 [v,u,w]

8 j .2.
(1) x,0,1/2 [u,0,0]
(2) x,0,1/2 [u,0,0]
(3) x,0,1/2 [u,0,0]
(4) x,0,1/2 [u,0,0]
(5) x,0,1/2 [u,0,0]
(6) x,0,1/2 [u,0,0]
(7) x,0,1/2 [u,0,0]
(8) x,0,1/2 [u,0,0]

8 i .2.
(1) x,0,0 [u,0,0]
(2) x,0,0 [u,0,0]
(3) x,0,0 [u,0,0]
(4) x,0,0 [u,0,0]
(5) x,0,0 [u,0,0]
(6) x,0,0 [u,0,0]
(7) x,0,0 [u,0,0]
(8) x,0,0 [u,0,0]

8 h .2
(1) x,x,0 [u,u,0]
(2) x,x,0 [u,u,0]
(3) x,x,0 [u,u,0]
(4) x,x,0 [u,u,0]
(5) x,x,0 [u,u,0]
(6) x,x,0 [u,u,0]
(7) x,x,0 [u,u,0]
(8) x,x,0 [u,u,0]

4 e 4..
(1) 1/2,0,z [0,0,w]
(2) 1/2,0,z [0,0,w]
(3) 1/2,0,z [0,0,w]
(4) 1/2,0,z [0,0,w]
(5) 1/2,0,z [0,0,w]
(6) 1/2,0,z [0,0,w]
(7) 1/2,0,z [0,0,w]
(8) 1/2,0,z [0,0,w]

4 d 4..’
(1) 1/2,0,1/4 [0,0,0]
(2) 1/2,0,1/4 [0,0,0]
(3) 1/2,0,1/4 [0,0,0]
(4) 1/2,0,1/4 [0,0,0]
(5) 1/2,0,1/4 [0,0,0]
(6) 1/2,0,1/4 [0,0,0]
(7) 1/2,0,1/4 [0,0,0]
(8) 1/2,0,1/4 [0,0,0]

2 b 422
(1) 0,0,1/2 [0,0,0]
(2) 0,0,1/2 [0,0,0]
(3) 0,0,1/2 [0,0,0]
(4) 0,0,1/2 [0,0,0]
(5) 0,0,1/2 [0,0,0]
(6) 0,0,1/2 [0,0,0]
(7) 0,0,1/2 [0,0,0]
(8) 0,0,1/2 [0,0,0]

2 a 422
(1) 0,0,0 [0,0,0]
(2) 0,0,0 [0,0,0]
(3) 0,0,0 [0,0,0]
(4) 0,0,0 [0,0,0]
(5) 0,0,0 [0,0,0]
(6) 0,0,0 [0,0,0]
(7) 0,0,0 [0,0,0]
(8) 0,0,0 [0,0,0]
Symmetry of Special Projections

Along [0,0,1] p4m' m' 
\[ a^* = (a - b)/2 \]
\[ b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] c 2m'm' 
\[ a^* = b \]
\[ b^* = c \]
Origin at x,0,0

Along [1,1,0] p 2m'm' 
\[ a^* = -(a + b)/2 \]
\[ b^* = c/2 \]
Origin at x,x,0
P4/mbm  
127.1.1053

4/mmm  
P4/m21/b2/m

Tetragonal

**Origin** at center (4/m) at 4/m121/g

**Asymmetric unit**
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

**Symmetry Operations**

(1) 1  
(1 | 0,0,0)

(2) 2  0,0,z  
(2_2 | 0,0,0)

(3) 4⁺  0,0,z  
(4 | 0,0,0)

(4) 4⁻  0,0,z  
(4_1 | 0,0,0)

(5) 2  (0,1/2,0)  1/4,y,0  
(2_1 | 1/2,1/2,0)

(6) 2  (1/2,0,0)  x,1/4,0  
(2_x | 1/2,1/2,0)

(7) 2  (1/2,1/2,0)  x,x,0  
(2_xy | 1/2,1/2,0)

(8) 2  x,x+1/2,0  
(2_xy | 1/2,1/2,0)

(9)  
(0,0,0)

(10) m  x,y,0  
(m_x | 0,0,0)

(11) 4⁺  0,0,z; 0,0,0  
(4 | 0,0,0)

(12) 4⁻  0,0,z; 0,0,0  
(4_1 | 0,0,0)

(13) a  (1/2,0,0)  x,1/4,z  
(m_y | 1/2,1/2,0)

(14) b  (0,1/2,0)  1/4,y,z  
(m_y | 1/2,1/2,0)

(15) m  x+1/2,x,z  
(m_y | 1/2,1/2,0)

(16) g  (1/2,1/2,0)  x,x,z  
(m_y | 1/2,1/2,0)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
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<tr>
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<td>m</td>
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<tr>
<td>2</td>
<td>a</td>
<td>4</td>
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</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1'  
Along [1,0,0] p\text{2\textast} 2\text{mm}  
Along [1,1,0] p2\text{mm}1'

\[ a^* = a \quad b^* = b \]  
\[ a^* = b/2 \quad b^* = c \]  
\[ a^* = (-a + b)/2 \quad b^* = c \]

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at x,x,0

127.1.1053 - 2 - 2158
Origin at center (4/m1') at 4/m12/,g1'

Asymmetric unit  
\[
0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad y \leq \frac{1}{2} - x
\]

Symmetry Operations

For 1 + set

1. \(1\)  
   \((1|0,0,0)\)

2. \(2\)  
   \((0,0,z)\)
   \((2_{z}|0,0,0)\)

3. \(4^+\)  
   \((0,0,z)\)
   \((4_{z}|0,0,0)\)

4. \(4^-\)  
   \((0,0,z)\)
   \((4_{z}^{-1}|0,0,0)\)

5. \(2\)  
   \((0,1/2,0)\)
   \((1/4,y,0)\)
   \((2_{y}|1/2,1/2,0)\)

6. \(2\)  
   \((1/2,0,0)\)
   \((x,1/4,0)\)
   \((2_{x}|1/2,1/2,0)\)

7. \(2\)  
   \((1/2,1/2,0)\)
   \((x,x,0)\)
   \((2_{xy}|1/2,1/2,0)\)

8. \(2\)  
   \((x,x+1/2,0)\)
   \((2_{xy}|1/2,1/2,0)\)

9. \(\overline{1}\)  
   \((0,0,0)\)
   \((1|0,0,0)\)

10. \(m\)  
    \((x,y,0)\)
    \((m_{x}|0,0,0)\)

11. \(4^+\)  
    \((0,0,z)\)
    \((0,0,0)\)
    \((4_{z}|0,0,0)\)

12. \(4^-\)  
    \((0,0,z)\)
    \((0,0,0)\)
    \((4_{z}^{-1}|0,0,0)\)

13. \(a\)  
    \((1/2,0,0)\)
    \((x,1/4,z)\)
    \((m_{x}|1/2,1/2,0)\)

14. \(b\)  
    \((0,1/2,0)\)
    \((1/4,y,z)\)
    \((m_{y}|1/2,1/2,0)\)

15. \(m\)  
    \((x+1/2,x,z)\)
    \((m_{x}|1/2,1/2,0)\)

16. \(g\)  
    \((1/2,1/2,0)\)
    \((x,x,z)\)
    \((m_{xy}|1/2,1/2,0)\)
Continued

For 1' + set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1'</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(2) 2'</td>
<td>x,y,z</td>
<td>[1/2,0,0]</td>
</tr>
<tr>
<td>(3) 4'</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(4) 4'</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(5) 2'</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
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<td>(6) 2'</td>
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<tr>
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<td>x,y,z</td>
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<td>[0,0,0]</td>
</tr>
<tr>
<td>(10) 1</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
</tr>
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<td>x,y,z</td>
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<td>(15) 1</td>
<td>x,y,z</td>
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</tr>
<tr>
<td>(16) 1</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
</tr>
</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.
2 b 4/m..1' 0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]
2 a 4/m..1' 0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4gm1'
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p 2mm1'
\[ a^* = b/2 \quad b^* = c \]
Origin at x,1/4,0

Along [1,1,0] p2mm1'
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,0
Origin at center (4/m') at 4/m'121'/g

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y < 1/2 - x

Symmetry Operations

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(3) 4+ 0,0,z
(4z|0,0,0)

(4) 4- 0,0,z
(4z|-1|0,0,0)

(5) 2' (0,1/2,0) 1/4,y,0
(2z|1/2,1/2,0)

(6) 2' (1/2,0,0) x,1/4,0
(2z|1/2,1/2,0)

(7) 2' (1/2,1/2,0) x,x,0
(2xy|1/2,1/2,0)

(8) 2' x,x+1/2,0
(2xy|1/2,1/2,0)

(9) 1' 0,0,0
(1|0,0,0)

(10) m' x,y,0
(mz|0,0,0)

(11) 4+ - 0,0,z; 0,0,0
(4z|0,0,0)

(12) 4- - 0,0,z; 0,0,0
(4z|-1|0,0,0)

(13) a (1/2,0,0) x,1/4,z
(mz|1/2,1/2,0)

(14) b (0,1/2,0) 1/4,y,z
(mz|1/2,1/2,0)

(15) m x+1/2,x,z
(mxy|1/2,1/2,0)

(16) g (1/2,1/2,0) x,x,z
(mxy|1/2,1/2,0)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
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</tr>
<tr>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
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</tr>
<tr>
<td>(2) x',y',z'</td>
<td>[u',v',w']</td>
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</tr>
<tr>
<td>(3) y,x,z</td>
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<tr>
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<td>(6) x+1/2,y+1/2,z'</td>
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<tr>
<td>(15) y+1/2,x+1/2,z</td>
<td>[v',u,w]</td>
<td></td>
</tr>
<tr>
<td>(16) y'+1/2,x'+1/2,z'</td>
<td>[v,u',w']</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p4gm
- Along [1,0,0] p2m'm'
- Along [1,1,0] p2mm1'

- Origin at 0,0,z
- Origin at x,0,0
- Origin at x,x,0
Origin at center (4'/m) at 4'/m121/g

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x \]

Symmetry Operations

1. \(1\) 
   \((0,0,0)\)

2. \(2\) 
   \((0,0,z)\) 
   \((2_z,0,0)\)

3. \(4^+\) 
   \((0,0,z)\) 
   \((4_z,0,0)\)

4. \(4^-\) 
   \((0,0,z)\) 
   \((4_z,0,0)\)

5. \(2'\) 
   \((0,1/2,0)\) 
   \((1/2,1/2,0)\)

6. \(2'\) 
   \((1/2,0,0)\) 
   \((1/4,y,0)\)

7. \(2\) 
   \((1/2,1/2,0)\) 
   \((2_x,1/4,y,0)\)

8. \(2\) 
   \((2_x,1/4,y,0)\)

9. \(\overline{1}\) 
   \((0,0,0)\)

10. \(m\) 
    \((x,y,0)\) 
    \((m_x,0,0)\)

11. \(\overline{4}^+\) 
    \((0,0,z)\) 
    \((4_z,0,0)\)

12. \(\overline{4}^-\) 
    \((0,0,z)\) 
    \((4_z,0,0)\)

13. \(a'\) 
    \((1/2,0,0)\) 
    \((x,1/4,z)\)

14. \(b'\) 
    \((0,1/2,0)\) 
    \((1/4,y,z)\)

15. \(m\) 
    \((x+1/2,\overline{1/2},0)\) 
    \((m_x,1/2,1/2,0)\)

16. \(g\) 
    \((1/2,1/2,0)\) 
    \((x,x,z)\)

127.4.1056 - 1 - 2164
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>l</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y, z [u, v, w]</td>
<td>(3) y, x, z [v, u, w]</td>
<td>(4) y, x, z [v, u, w]</td>
</tr>
<tr>
<td>(5) x+1/2, y+1/2, z [u, v, w]</td>
<td>(6) x+1/2, y+1/2, z [u, v, w]</td>
<td>(7) y+1/2, x+1/2, z [v, u, w]</td>
<td>(8) y+1/2, x+1/2, z [v, u, w]</td>
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<tr>
<td>(9) x, y, z [u, v, w]</td>
<td>(10) x, y, z [u, v, w]</td>
<td>(11) y, x, z [v, u, w]</td>
<td>(12) y, x, z [v, u, w]</td>
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<tr>
<td>(13) x+1/2, y+1/2, z [u, v, w]</td>
<td>(14) x+1/2, y+1/2, z [u, v, w]</td>
<td>(15) y+1/2, x+1/2, z [v, u, w]</td>
<td>(16) y+1/2, x+1/2, z [v, u, w]</td>
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8 k m

<table>
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<tr>
<th>8</th>
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<tbody>
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<td>x, y, 1/2 [0, 0, w]</td>
<td>x, y, 1/2 [0, 0, w]</td>
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<tr>
<td>x+1/2, y+1/2, 1/2 [0, 0, w]</td>
<td>x+1/2, y+1/2, 1/2 [0, 0, w]</td>
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8 i m

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<td>x+1/2, y+1/2, 0 [0, 0, w]</td>
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<tr>
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<td>y, x, 0 [0, 0, w]</td>
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4 h m2m

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<tr>
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<tr>
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<td>x, x+1/2, 1/2 [0, 0, 0]</td>
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<tr>
<td>x+1/2, y+1/2, 0 [0, 0, w]</td>
<td>x+1/2, y+1/2, 0 [0, 0, w]</td>
<td>x+1/2, y+1/2, 0 [0, 0, w]</td>
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<tr>
<td>y, x, 0 [0, 0, w]</td>
<td>y, x, 0 [0, 0, w]</td>
<td>y, x, 0 [0, 0, w]</td>
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4 g m2m

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<th>m2m</th>
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</thead>
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<td>x, x+1/2, 0 [0, 0, 0]</td>
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4 f 2.mm

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<tr>
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<tr>
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</table>

4 e 4'..

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<tr>
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<th>e</th>
<th>4'..</th>
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<tbody>
<tr>
<td>0, 0, z [0, 0, 0]</td>
<td>1/2, 1/2, z [0, 0, 0]</td>
<td>1/2, 1/2, z [0, 0, 0]</td>
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<tr>
<td>1/2, 1/2, z [0, 0, 0]</td>
<td>1/2, 1/2, z [0, 0, 0]</td>
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2 d m.mm

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<tr>
<th>2</th>
<th>d</th>
<th>m.mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 1/2, 0 [0, 0, 0]</td>
<td>1/2, 0, 0 [0, 0, 0]</td>
<td>1/2, 0, 0 [0, 0, 0]</td>
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2 c m.mm

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<tr>
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<th>m.mm</th>
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</thead>
<tbody>
<tr>
<td>0, 1/2, 1/2 [0, 0, 0]</td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
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</table>

2 b 4'm..

<table>
<thead>
<tr>
<th>2</th>
<th>b</th>
<th>4'm..</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 0, 1/2 [0, 0, 0]</td>
<td>1/2, 1/2, 1/2 [0, 0, 0]</td>
<td>1/2, 1/2, 1/2 [0, 0, 0]</td>
</tr>
</tbody>
</table>

2 a 4'm..

<table>
<thead>
<tr>
<th>2</th>
<th>a</th>
<th>4'm..</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 0, 0 [0, 0, 0]</td>
<td>1/2, 1/2, 0 [0, 0, 0]</td>
<td>1/2, 1/2, 0 [0, 0, 0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
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<tr>
<th>Along [0,0,1]</th>
<th>p4gm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2'2'2m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c</td>
<td>b* = b/2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p22m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -(a + b)/2</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,0,0

Origin at x,x,0
**Origin** at center (4'/m) at 4'/m121'/g'

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

**Symmetry Operations**

(1) 1

(2) 2 0,0,z

(3) 4' 0,0,z

(4) 4' 0,0,z

(5) 2 (0,1/2,0) 1/4,y,0

(6) 2 (1/2,0,0) x,1/4,0

(7) 2' (1/2,1/2,0) x,x,0

(8) 2' x,x+1/2,0

(9) 1 0,0,0

(10) m x,y,0

(11) 4' 0,0,z; 0,0,0

(12) 4' 0,0,z; 0,0,0

(13) a (1/2,0,0) x,1/4,z

(14) b (0,1/2,0) 1/4,y,z

(15) m' x+1/2,x,z

(16) g' (1/2,1/2,0) x,x,z
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

16  l  1

(1) x,y,z [u,v,w]  (2) x,\bar{y},z [\bar{u},v,\bar{w}]  (3) \bar{y},x,z [v,u,\bar{w}]  (4) y,\bar{x},z [v,u,\bar{w}]

(5) x+1/2,y+1/2,z [\bar{u},v,\bar{w}]  (6) x+1/2,\bar{y}+1/2,z [u,v,\bar{w}]  (7) y+1/2,x+1/2,z [v,u,\bar{w}]  (8) \bar{y}+1/2,\bar{x}+1/2,z [v,u,\bar{w}]

(9) \bar{x},y,z [u,v,\bar{w}]  (10) x,y,z [u,v,\bar{w}]  (11) y,\bar{x},z [v,u,\bar{w}]  (12) \bar{y},x,\bar{z} [v,u,\bar{w}]

(13) x+1/2,\bar{y}+1/2,z [u,v,\bar{w}]  (14) x+1/2,y+1/2,z [u,\bar{v},\bar{w}]  (15) y+1/2,\bar{x}+1/2,z [u,\bar{v},\bar{w}]  (16) y+1/2,x+1/2,z [v,u,\bar{w}]

8  k  ..m'  x,x+1/2,z [u,u,\bar{w}]  \bar{x},x+1/2,z [\bar{u},u,\bar{w}]  \bar{x},\bar{x}+1/2,z [u,\bar{u},\bar{w}]  x+1/2,\bar{x},z [u,u,\bar{w}]

x+1/2,x,\bar{z} [u,u,\bar{w}]  x+1/2,x,z [u,u,\bar{w}]  x,x+1/2,z [u,u,\bar{w}]  \bar{x},x+1/2,z [u,u,\bar{w}]

8  j  m..  x,y,1/2 [0,0,w]  x,\bar{y},1/2 [0,0,w]  \bar{y},x,1/2 [0,0,w]  y,\bar{x},1/2 [0,0,w]

\bar{x}+1/2,y+1/2,1/2 [0,0,w]  x+1/2,\bar{y}+1/2,1/2 [0,0,w]  y+1/2,\bar{x}+1/2,1/2 [0,0,w]  \bar{y}+1/2,\bar{x}+1/2,1/2 [0,0,w]

8  i  m..  x,y,0 [0,0,w]  x,\bar{y},0 [0,0,w]  \bar{y},x,0 [0,0,w]  y,\bar{x},0 [0,0,w]

\bar{x}+1/2,y+1/2,0 [0,0,w]  x+1/2,\bar{y}+1/2,0 [0,0,w]  y+1/2,\bar{x}+1/2,0 [0,0,w]  \bar{y}+1/2,\bar{x}+1/2,0 [0,0,w]

4  h  m.2'm'  x,x+1/2,1/2 [0,0,w]  x,\bar{x}+1/2,1/2 [0,0,w]  \bar{x}+1/2,\bar{x},1/2 [0,0,w]  x+1/2,\bar{x},1/2 [0,0,w]

4  g  m.2'm'  x,x+1/2,0 [0,0,w]  x,\bar{x}+1/2,0 [0,0,w]  \bar{x}+1/2,\bar{x},0 [0,0,w]  x+1/2,\bar{x},0 [0,0,w]

4  f  2.m.m'  0,1/2,z [0,0,w]  1/2,0,z [0,0,\bar{w}]  1/2,0,\bar{z} [0,0,w]  0,1/2,\bar{z} [0,0,w]

4  e  4'..  0,0,z [0,0,0]  1/2,1/2,z [0,0,0]  0,0,\bar{z} [0,0,0]  1/2,1/2,\bar{z} [0,0,0]

2  d  m.m.m'  0,1/2,0 [0,0,w]  1/2,0,0 [0,0,w]

2  c  m.m.m'  0,1/2,1/2 [0,0,w]  1/2,0,1/2 [0,0,w]

2  b  4'/m..  0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]

2  a  4'/m..  0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4gm1'  Along [1,0,0]  p2a  2mm  Along [1,1,0]  p2'2mm'  
a^* = a  \ b^* = b  \ a^* = b/2  \ b^* = c  \ a^* = -c  \ b^* = (-a + b)/2

Origin at 0,0,z  \ Origin at x,1/4,0  \ Origin at x,x,0
Origin at center (4'/m') at 4'/m'121'/g

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

(1) 1 (1|0,0,0)
(2) 2 0,0,z (2z|0,0,0)
(3) 4+ 0,0,z (4z|0,0,0)'
(4) 4- 0,0,z (4z|0,0,0)'
(5) 2 (0,1/2,0) 1/4,y,0 (2z|1/2,1/2,0)
(6) 2 (1/2,0,0) x,1/4,0 (2z|1/2,1/2,0)
(7) 2' (1/2,1/2,0) x,x,0 (2xy|1/2,1/2,0)'
(8) 2' x,x +1/2,0 (2xy|1/2,1/2,0)'
(9) T 0,0,0 (T|0,0,0)'
(10) m' x,y,0 (mz|0,0,0)'
(11) 4+ 0,0,z; 0,0,0 (4z|0,0,0)
(12) 4- 0,0,z; 0,0,0 (4z|0,0,0)'
(13) a' (1/2,0,0) x,1/4,z (mz|1/2,1/2,0)'
(14) b' (0,1/2,0) 1/4,y,z (mz|1/2,1/2,0)'
(15) m x+1/2,x,z (mx|1/2,1/2,0)
(16) g (1/2,1/2,0) x,x,z (mx|1/2,1/2,0)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<td>l</td>
<td>1</td>
</tr>
</tbody>
</table>

(1) x,y,z [u,v,w]  
(2) x,y,z [u,v,w]  
(3) y,x,z [v,u,w]  
(4) y,x,z [v,u,w]

(5) x+1/2,y+1/2,z [u,v,w]  
(6) x+1/2,y+1/2,z [u,v,w]  
(7) y+1/2,x+1/2,z [v,u,w]  
(8) y+1/2,x+1/2,z [v,u,w]

(9) x,y,z [u,v,w]  
(10) x,y,z [u,v,w]  
(11) y,x,z [v,u,w]  
(12) y,x,z [v,u,w]

(13) x+1/2,y+1/2,z [u,v,w]  
(14) x+1/2,y+1/2,z [u,v,w]  
(15) y+1/2,x+1/2,z [v,u,w]  
(16) y+1/2,x+1/2,z [v,u,w]

### Coordinates

<p>| | | | | |</p>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4g'm</th>
<th>Along [1,0,0]</th>
<th>p2mm'</th>
<th>Along [1,1,0]</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = (a + b)/2</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at x,x,0
Origin at center (4/m) at 4/m121'/g'

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad y \leq \frac{1}{2} - x \]

Symmetry Operations

1. \((1 | 0,0,0)\)
2. \((2 | 0,0,z) (2_z | 0,0,0)\)
3. \(4^+ 0,0,z (4_z | 0,0,0)\)
4. \(4^- 0,0,z (4_z^{-1} | 0,0,0)\)
5. \(2' (0,1/2,0) 1/4,y,0 (2_z, 1/2,1/2,0)'\)
6. \(2' (1/2,0,0) x,1/4,0 (2_z, 1/2,1/2,0)'\)
7. \(2' (1/2,1/2,0) x,x,0 (2_{xy}, 1/2,1/2,0)'\)
8. \(2' x, x+1/2,0 (2_{xy}, 1/2,1/2,0)'\)
9. \(\tilde{1} 0,0,0 (1 | 0,0,0)\)
10. \(m x,y,0 (m_z | 0,0,0)\)
11. \(4^+ 0,0,z; 0,0,0 (4_z | 0,0,0)\)
12. \(4^- 0,0,z; 0,0,0 (4_z^{-1} | 0,0,0)\)
13. \(a' (1/2,0,0) x,1/4,z (m_z, 1/2,1/2,0)'\)
14. \(b' (0,1/2,0) 1/4,y,z (m_{xy}, 1/2,1/2,0)'\)
15. \(m' x+1/2,\bar{x},z (m_{xy}, 1/2,1/2,0)'\)
16. \(g' (1/2,1/2,0) x, x,z (m_{xy}, 1/2,1/2,0)'\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions  

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<td>2</td>
<td>b</td>
<td>4/m..</td>
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<tr>
<td>Symmetry of Special Projections</td>
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</tbody>
</table>

Along [0,0,1]  
p4gm1'  
a* = a  b* = b
Origin at 0,0,z

Along [1,0,0]  
p2'2'm'

Along [1,1,0]  
p22'nm'

Along [1,1,0]  
p22'nm'

a* = -c  b* = (-a + b)/2
Origin at x,x,0
**Origin** at center (4'/m') at 4'/m'121/g'

**Asymmetric unit**

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad y \leq \frac{1}{2} - x\]

**Symmetry Operations**

1. \(1 (0,0,0)\)
2. \(2 (0,0,z) (\frac{1}{2},0,0)\)
3. \(4' (0,0,z) (\frac{1}{2},0,0)'\)
4. \(4' (0,0,z) (\frac{1}{2},0,0)'\)
5. \(2' (0,1/2,0) (1,1/2,0)'\)
6. \(2' (1/2,0,0) (1,1/2,0)'\)
7. \(2 (1/2,1/2,0) (1,1/2,0)'\)
8. \(2 (1/2,1/2,0) (1,1/2,0)'\)
9. \(\bar{1} (0,0,0)\)
10. \(m' (x,y,0) (m_z,0,0)'\)
11. \(\bar{4} (x,y,0) (m_z,0,0)'\)
12. \(\bar{4} (x,y,0) (m_z,0,0)'\)
13. \(a (x,y,0) (m_z,1/2,1/2,0)\)
14. \(b (0,1/2,0) (1/2,1/2,0)'\)
15. \(m' (x+1/2,x,z) (m_{xy},1/2,1/2,0)'\)
16. \(g' (x,y,z) (m_{xy},1/2,1/2,0)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
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</table>

(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y,x,z [v,u,w]  (4) y,x,z [v,u,w]  (5) x+1/2,y+1/2,z [u,v,w]  (6) x+1/2,y+1/2,z [u,v,w]  (7) y+1/2,x+1/2,z [v,u,w]  (8) y+1/2,x+1/2,z [v,u,w]  (9) x,y,z [u,v,w]  (10) x,y,z [u,v,w]  (11) y,x,z [v,u,w]  (12) y,x,z [v,u,w]  (13) x+1/2,y+1/2,z [u,v,w]  (14) x+1/2,y+1/2,z [u,v,w]  (15) y+1/2,x+1/2,z [v,u,w]  (16) y+1/2,x+1/2,z [v,u,w]

8 | k | .m' |
---|---|-----|
| x,x+1/2,z [u,u,w] | x,x+1/2,z [u,u,w] | x+1/2,x,z [u,u,w] | x+1/2,x,z [u,u,w] |
| x+1/2,y+1/2,z [u,u,w] | x+1/2,y+1/2,z [u,u,w] | x,x+1/2,z [u,u,w] | x,x+1/2,z [u,u,w] |

8 | j | m'. | |
---|---|----|---|
| x,y,1/2 [u,v,0] | x,y,1/2 [u,v,0] | y,x,1/2 [v,u,0] | y,x,1/2 [v,u,0] |
| x+1/2,y+1/2,1/2 [u,v,0] | x+1/2,y+1/2,1/2 [u,v,0] | y+1/2,x+1/2,1/2 [v,u,0] | y+1/2,x+1/2,1/2 [v,u,0] |

8 | i | m'. | |
---|---|----|---|
| x,y,0 [u,v,0] | x,y,0 [u,v,0] | y,x,0 [v,u,0] | y,x,0 [v,u,0] |
| x+1/2,y+1/2,0 [u,v,0] | x+1/2,y+1/2,0 [u,v,0] | y+1/2,x+1/2,0 [v,u,0] | y+1/2,x+1/2,0 [v,u,0] |

4 | h | m'.2m' |
---|---|------|
| x,x+1/2,1/2 [u,u,0] | x,x+1/2,1/2 [u,u,0] | x+1/2,x,1/2 [u,u,0] | x+1/2,x,1/2 [u,u,0] |

4 | g | m'.2m' |
---|---|------|
| x,x+1/2,0 [u,u,0] | x,x+1/2,0 [u,u,0] | x+1/2,x,0 [u,u,0] | x+1/2,x,0 [u,u,0] |

4 | f | 2.m'm' |
---|---|------|
| 0,1/2,z [0,0,w] | 0,1/2,z [0,0,w] | 1/2,0,z [0,0,w] | 1/2,0,z [0,0,w] |

4 | e | 4'.. |
---|---|-----|
| 0,0,z [0,0,0] | 0,0,z [0,0,0] | 0,0,z [0,0,0] | 0,0,z [0,0,0] |

2 | d | m'.m'm' |
---|---|-----|
| 0,1/2,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,0,0 [0,0,0] | 1/2,0,0 [0,0,0] |

2 | c | m'.m'm' |
---|---|-----|
| 0,1/2,1/2 [0,0,0] | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |

2 | b | 4'/m'.. |
---|---|-----|
| 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 1/2,1,2,1/2 [0,0,0] | 1/2,1,2,1/2 [0,0,0] |

2 | a | 4'/m'.. |
---|---|-----|
| 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 1/2,1,2,0 [0,0,0] | 1/2,1,2,0 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1]  p4'gm'  Along [1,0,0]  p2m'm'  Along [1,1,0]  p2m'm'

a* = a  b* = b  a* = b/2  b* = c  a* = -(a + b)/2  b* = c

Origin at 0,0,z  Origin at x,1/4,0  Origin at x,x,0
Origin at center (4/m') at 4/m'121/g'

Asymmetric unit

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad y \leq \frac{1}{2} - x\]

Symmetry Operations

1. \(1 \rightarrow (1|0,0,0)\)
2. \(2 \rightarrow (0,0,z) (2z|0,0,0)\)
3. \(4^+ \rightarrow (0,0,z) (4z|0,0,0)\)
4. \(4^- \rightarrow (0,0,z) (4z|0,0,0)\)
5. \(2 \rightarrow (0,1/2,0) \rightarrow (1/2,0,0) \rightarrow (1/2,1/2,0) \rightarrow (1,0,0)\)
6. \(2 \rightarrow (1/2,0,0) \rightarrow (1,0,0)\)
7. \(2 \rightarrow (1/2,1/2,0) \rightarrow (1,0,0)\)
8. \(2 \rightarrow (1/2,1/2,0) \rightarrow (1,0,0)\)
9. \(3 \rightarrow (0,0,0)\)
10. \(m' \rightarrow (m|0,0,0)\)
11. \(4^+ \rightarrow (0,0,z) (4z|0,0,0)\)
12. \(4^- \rightarrow (0,0,z) (4z|0,0,0)\)
13. \(a' \rightarrow (1/2,0,0) \rightarrow (1,0,0)\)
14. \(b' \rightarrow (0,1/2,0) \rightarrow (1,0,0)\)
15. \(m' \rightarrow (m|0,0,0)\)
16. \(g' \rightarrow (1/2,1/2,0) \rightarrow (1,0,0)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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Symmetry of Special Projections

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<td>b* = c</td>
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<td>Origin at x,1/4,0</td>
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<th>p2m'm'</th>
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<td>a* = (-a + b)/2</td>
<td>b* = c</td>
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<td>Origin at x,x,0</td>
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</table>

127.9.1061 - 2 - 2175
Origin at center (4/m) at 4/m 121/g

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1  
(1*0,0,0) 

(2) 2 0,0,0  
(2z,0,0) 

(3) 4* 0,0,0  
(4z,0,0,0) 

(4*) 0,0,0  
(4z*0,0,0) 

(5) 2 (0.1/2,0) 1/4,y,0  
(2z,1/2,1/2,0) 

(6) 2 (1/2,0,0) x,1/4,0  
(2z,1/2,1/2,0) 

(7) 2 (1/2,1/2,0) x,x,0  
(2xy,1/2,1/2,0) 

(8) 2 x,x+1/2,0  
(2xy,1/2,1/2,0) 

(9) 1 0,0,0  
(10) m x,y,0  
(mz,0,0,0) 

(11) 4* 0,0,0; 0,0,0  
(4z,0,0,0) 

(12) 4* 0,0,0; 0,0,0  
(4z*0,0,0) 

(13) a (1/2,0,0) 1/4,y,z  
(mz,1/2,1/2,0) 

(14) b (0,1/2,0) 1/4,y,z  
(mz,1/2,1/2,0) 

Generators selected (1); t(0,0,0); t(0,0,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

(0,0,0) +  

Coordinates

16 k .m  

(0,0,0) +  

(0,0,0)^' +  

16 k .m  

127.10.1062 - 2 - 2177
Symmetry of Special Projections

Along [0,0,1] p4gm1'  
Along [1,0,0]  p2mm  
Along [1,1,0]  p2mm1'  

a* = a  b* = b  
Origin at 0,0,z  

a* = b/2  b* = c  
Origin at x,1/4,0  

a* = (-a + b)/2  b* = c  
Origin at x,x,0
$P_2c \ 4'/mb'm$

$4/mmm1'$

Tetragonal

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$P_2c \ 4'/m21'/b'2/m$
Origin at center (4/m) at 4/m12, /g

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 0,0,z (2z|0,0,0)
(3) 4+ 0,0,z (4z|0,0,0)
(4) 4+ 0,0,z
(5) 2 (0,1/2,0) 1/4,y,0 (2z|1/2,1/2,0)
(6) 2' (1/2,0,0) x,1/4,0 (2z|1/2,1/2,0)
(7) 2 (1/2,1/2,0) x,x,0 (2z|1/2,1/2,0)
(8) 2 x,x+1/2,0
(9) 3 0,0,0
(10) m x,y,0 (m|0,0,0)
(11) 4+ 0,0,z; 0,0,0 (4z|0,0,0)
(12) 4+ 0,0,z; 0,0,0
(13) a' (1/2,0,0) x,1/4,z (m|1/2,1/2,0)
(14) b' (0,1/2,0) 1/4,y,z (m|1/2,1/2,0)
(15) g (1/2,1/2,0) x,x,z
(16) g' (1/2,1/2,0) x,x,z

For (0,0,1) ' set

(1) t' (0,0,1)
(2) 2' (0,0,1) 0,0,z (2z|0,0,1)
(3) 4+ (0,0,1) 0,0,z
(4) 4+ (0,0,1) 0,0,z
(5) 2 (0,1/2,0) 1/4,y,1/2 (2z|1/2,1/2,1)
(6) 2' (1/2,0,0) x,1/4,1/2 (2z|1/2,1/2,1)
(7) 2 (1/2,1/2,0) x,x,1/2 (2z|1/2,1/2,1)
(8) 2' x,x+1/2,1/2
(9) 3 0,0,1/2
(10) m' x,y,1/2 (m|0,0,1)
(11) 4+ 0,0,z; 0,0,1/2
(12) 4+ 0,0,z; 0,0,1/2
(13) n (1/2,0,1) x,1/4,z (m|1/2,1/2,1)
(14) n (0,1/2,1) 1/4,y,z (m|1/2,1/2,1)
(15) c' (0,0,1) x+1/2, x,z (m|1/2,1/2,1)
(16) n' (1/2,1/2,1) x,x,z

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) +
(0,0,1) +

32 l 1

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) y,x,z [v,u,w]
(4) y,x,z [v,u,w]

(5) x+1/2,y+1/2,z [u,v,w]
(6) x+1/2,y+1/2,z [u,v,w]
(7) y+1/2,x+1/2,z [v,u,w]
(8) y+1/2,x+1/2,z [v,u,w]

(9) x,y,z [u,v,w]
(10) x,y,z [u,v,w]
(11) y,x,z [v,u,w]
(12) y,x,z [v,u,w]

(13) x+1/2,y+1/2,z [u,v,w]
(14) x+1/2,y+1/2,z [u,v,w]
(15) y+1/2,x+1/2,z [v,u,w]
(16) y+1/2,x+1/2,z [v,u,w]

16 k .m x,x+1/2,z [u,u,0] x,x+1/2,z [u,u,0] x,x+1/2,z [u,u,0] x,x+1/2,z [u,u,0]

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**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [1,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p4gm1'</td>
<td>0,0,z</td>
<td>a* = a</td>
<td>a* = -c, b* = b/2</td>
<td>a* = (-a + b)/2</td>
</tr>
<tr>
<td>p 2'mm'</td>
<td>x,0</td>
<td>a* = a</td>
<td>a* = -c, b* = b/2</td>
<td>a* = (-a + b)/2</td>
</tr>
<tr>
<td>p2mm1'</td>
<td>x,x,0</td>
<td>a* = a</td>
<td>a* = -c, b* = b/2</td>
<td>a* = (-a + b)/2</td>
</tr>
</tbody>
</table>

**Origin at**
- 0,0,z
- x,0
- x,x,0
$P_{2c} 4'/mbm'$

127.12.1064

$4/mmm1'$

$P_{2c} 4'/m2',/b2'/m'$

Tetragonal
Continued

Origin at center (4/m) at 4/m121'/g

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1  (2) 2 0,0,z  (3) 4+ 0,0,z  (4) 4' 0,0,z  (4') 0,0,0'  (4'') 0,0,0''

(1) 0,0,0  (2) 0,0,0  (3) 0,0,0  (4) 0,0,0'  (4') 0,0,0''  (4'') 0,0,0'''

(5) 2 0,1/2,0 1/4,y,0  (6) 2 0,1/2,0 1/4,y,0  (7) 2' 0,1/2,0 1/4,y,0  (8) 2' 0,1/2,0 1/4,y,0
(2z, 1/2,1/2,0)  (2z, 1/2,1/2,0)  (2x, 1/2,1/2,0)  (2x, 1/2,1/2,0)

(9) 0,0,0  (10) m x,y,0  (11) 4+z 0,0,0  (12) 4+z 0,0,0  (4+z) 0,0,0 (4+z) 0,0,0'

(13) a 0,1/2,0 1/4,y,z  (m, 1/2,1/2,0)  (14) b 0,1/2,0 1/4,y,z  (m, 1/2,1/2,0)  (15) m' x+1/2,x,z  (m, 1/2,1/2,0)

For (0,0,1) + set

(1) t 0,0,0  (2) 2 0,0,0  (3) 4- 0,0,0  (4) 4- 0,0,0  (4) 0,0,0,0  (4) 0,0,0,0

(1) 0,0,0  (2) 0,0,0  (3) 0,0,0  (4) 0,0,0  (4) 0,0,0  (4) 0,0,0

(5) 2 0,1/2,0 1/4,y,1/2  (6) 2' 0,1/2,0 1/4,y,1/2  (7) 2' 0,1/2,0 1/4,y,1/2  (8) 2' 0,1/2,0 1/4,y,1/2
(2z, 1/2,2/1,0)  (2z, 1/2,2/1,0)  (2z, 1/2,2/1,0)  (2z, 1/2,2/1,0)

(9) 0,0,1/2  (10) m' x,y,1/2  (11) 4- 0,0,1/2  (12) 4- 0,0,1/2  (4-') 0,0,1/2  (4-') 0,0,1/2

(13) n 0,1/2,0 1/4,y,z  (m, 1/2,1/2,1)  (14) n' 0,1/2,0 1/4,y,z  (m, 1/2,1/2,1)  (15) c 0,0,1/2 x+1/2,x,z  (m, 1/2,1/2,1)

Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' +</td>
<td></td>
</tr>
</tbody>
</table>

32 1 1

(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) y,x,z [v,u,w]  (4) y,x,z [v,u,w]

(5) x+1/2,y+1/2,z [u,v,w]  (6) x+1/2,y+1/2,z [u,v,w]  (7) y+1/2,x+1/2,z [v,u,w]  (8) y+1/2,x+1/2,z [v,u,w]

(9) x,y,z [u,v,w]  (10) x,y,z [u,v,w]  (11) y,x,z [v,u,w]  (12) y,x,z [v,u,w]

(13) x+1/2,y+1/2,z [u,v,w]  (14) x+1/2,y+1/2,z [u,v,w]  (15) y+1/2,x+1/2,z [v,u,w]  (16) y+1/2,x+1/2,z [v,u,w]

16 k ..m' x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]  x,x+1/2,z [u,u,w]

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Continued

16  j  m'..  x,y,1/2 [u,v,0]  \bar{x},\bar{y},1/2 [\bar{u},\bar{v},0]  \bar{y},x,1/2 [v,\bar{u},0]  y,\bar{x},1/2 [\bar{v},u,0]  
   \bar{x}+1/2,y+1/2,1/2 [u,\bar{v},0]  x+1/2,y+1/2,1/2 [\bar{u},v,0]  y+1/2,x+1/2,1/2 [v,u,0]  \bar{y}+1/2,\bar{x}+1/2,1/2 [\bar{v},u,0] 

16  i  m..  x,y,0 [0,0,w]  \bar{x},\bar{y},0 [0,0,w]  \bar{y},x,0 [0,0,w]  y,\bar{x},0 [0,0,w]  
   \bar{x}+1/2,y+1/2,0 [0,0,\bar{w}]  x+1/2,\bar{y}+1/2,0 [0,0,\bar{w}]  y+1/2,x+1/2,0 [0,0,\bar{w}]  \bar{y}+1/2,\bar{x}+1/2,0 [0,0,\bar{w}] 

8   h  m'.2m'  x,x+1/2,1/2 [u,u,0]  \bar{x},x+1/2,1/2 [\bar{u},\bar{u},0]  \bar{x}+1/2,\bar{x},1/2 [u,\bar{u},0]  x+1/2,\bar{x},1/2 [\bar{u},u,0] 

8   g  m.2'm'  x,x+1/2,0 [0,0,w]  \bar{x},x+1/2,0 [0,0,\bar{w}]  \bar{x}+1/2,\bar{x},0 [0,0,\bar{w}]  x+1/2,\bar{x},0 [0,0,\bar{w}] 

8   f  2.m'm'  0,1/2,z [0,0,w]  1/2,0,z [0,0,\bar{w}]  1/2,0,z [0,0,\bar{w}]  0,1/2,z [0,0,\bar{w}] 

8   e  4'..  0,0,z [0,0,0]  1/2,1/2,z [0,0,0]  0,0,z [0,0,0]  1/2,1/2,z [0,0,0] 

4   d  m.m'm'  0,1/2,0 [0,0,w]  1/2,0,0 [0,0,\bar{w}] 

4   c  m'.mm  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0] 

4   b  4'/m'..  0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0] 

4   a  4'/m..  0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0] 

Symmetry of Special Projections

Along $[0,0,1]$  \text{p4gm1}^*$  Along $[1,0,0]$  \text{p}_{\text{cm}} 2\text{mm}  Along $[1,1,0]$  \text{p}_{2\text{cm}} 2\text{m}'\text{m}' 
\begin{align*}
\text{a}^* &= \text{a} & \text{b}^* &= \text{b} & \text{a}^* &= \text{b}/2 & \text{b}^* &= \text{c} & \text{a}^* &= -\text{c} & \text{b}^* &= (-\text{a} + \text{b})/2 \\
\text{Origin at} 0,0,z & & \text{Origin at} x,1/4,0 & & \text{Origin at} x,x,1/2
\end{align*}
P2c 4/mbm'  
127.13.1065  
P2c 4/m21'/b'2'/m'  
4/mmm1'  
Tetragonal
Origin at center (4/m) at 4/m121'/g'

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2; \quad y < 1/2 - x \]

Symmetry Operations

For \((0,0,0)\) + set

(1) \(1 \) (1 | 0,0,0)
(2) \(2 \) 0,0,z
(3) \(4^* \) 0,0,z
(4) \(4^* \) 0,0,z

(5) \(2' \) (0,1/2,0) 1/4,y,0
(6) \(2' \) (1/2,1/2,0) x,1/4,0
(7) \(2' \) (1/2,1/2,0) x,x,0
(8) \(2' \) x,x+1/2,0

(9) \(\overline{1} \) 0,0,0
(10) m x,y,0
(11) \(4^* \) 0,0,z; 0,0,0
(12) \(4^* \) 0,0,z; 0,0,0

(13) \(a' \) (1/2,0,0) x,1/4,z
(14) \(b' \) (0,1/2,0) 1/4,y,z
(15) m' x+1/2,\overline{x},z
(16) g' (1/2,1/2,0) x,x,z

For \((0,0,1)\)' + set

(1) \(t' \) (0,0,1)
(2) \(2' \) (0,0,1) 0,0,z
(3) \(4^* \) (0,0,1) 0,0,z
(4) \(4^* \) (0,0,1) 0,0,z

(5) \(2 \) (0,1/2,0) 1/4,y,1/2
(6) \(2 \) (1/2,1/2,1) x,1/4,1/2
(7) \(2 \) (1/2,1/2,1) x,x,1/2
(8) \(2 \) x,x+1/2,1/2

(9) \(\overline{1} \) 0,0,1/2
(10) m' x,y,1/2
(11) \(4^* \) 0,0,z; 0,0,1/2
(12) \(4^* \) 0,0,z; 0,0,1/2

(13) \(n \) (1/2,0,1) x,1/4,z
(14) \(n \) (0,1/2,1) 1/4,y,z
(15) c (0,0,1) x+1/2,\overline{x},z
(16) n (1/2,1/2,1) x,x,z

Generators selected

(1); \(t(1,0,0); \) \(t(0,1,0); \) \(t'(0,0,1); \) (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>(0,0,0) +</th>
<th>(0,0,1)' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z ([u,v,w] )</td>
<td>(x,\overline{y},z ) ([\overline{u},\overline{v},w] )</td>
</tr>
<tr>
<td>(5) (x+1/2,\overline{y}+1/2,\overline{z} ) ([u,\overline{v},w] )</td>
<td>(x+1/2,\overline{y}+1/2,\overline{z} ) ([u,\overline{v},w] )</td>
</tr>
<tr>
<td>(9) (x,\overline{y},z ) ([u,v,w] )</td>
<td>(x,y,\overline{z} ) ([u,\overline{v},\overline{w}] )</td>
</tr>
<tr>
<td>(13) (x+1/2,\overline{y}+1/2,\overline{z} ) ([u,\overline{v},\overline{w}] )</td>
<td>(x+1/2,\overline{y}+1/2,\overline{z} ) ([u,\overline{v},\overline{w}] )</td>
</tr>
</tbody>
</table>

16 \(k \) \(m' \) \(x,x+1/2,\overline{z} \) \([u,u,w] \) | \(x,x+1/2,\overline{z} \) \([u,u,w] \) | \(x,x+1/2,\overline{z} \) \([u,u,w] \) | \(x,x+1/2,\overline{z} \) \([u,u,w] \) |
Continued

16 j m'. x,y,1/2 [u,v,0] \( \bar{x},\bar{y},1/2 [\bar{u},\bar{v},0] \) \( \bar{y},x,1/2 [\bar{v},u,0] \) \( y,\bar{x},1/2 [v,\bar{u},0] \)
\( \bar{x}+1/2,y+1/2,1/2 [\bar{u},\bar{v},0] \) \( x+1/2,\bar{y}+1/2,1/2 [u,\bar{v},0] \) \( y+1/2,x+1/2,1/2 [v,u,0] \) \( \bar{y}+1/2,\bar{x}+1/2,1/2 [\bar{v},\bar{u},0] \)

16 i m.. x,y,0 [0,0,w] \( \bar{x},\bar{y},0 [0,0,w] \) \( \bar{y},x,0 [0,0,w] \) \( y,\bar{x},0 [0,0,w] \)
\( \bar{x}+1/2,y+1/2,0 [0,0,w] \) \( x+1/2,\bar{y}+1/2,0 [0,0,w] \) \( y+1/2,x+1/2,0 [0,0,w] \) \( \bar{y}+1/2,\bar{x}+1/2,0 [0,0,w] \)

8 h m'.2m' x,x+1/2,1/2 [u,u,0] \( \bar{x},\bar{x}+1/2,1/2 [\bar{u},\bar{u},0] \) \( \bar{x}+1/2,\bar{x},1/2 [\bar{u},\bar{u},0] \) \( x+1/2,\bar{x},1/2 [u,\bar{u},0] \)

8 g m.2' m' x,x+1/2,0 [0,0,w] \( \bar{x},\bar{x}+1/2,0 [0,0,w] \) \( \bar{x}+1/2,\bar{x},0 [0,0,w] \) \( x+1/2,\bar{x},0 [0,0,w] \)

8 f 2.m'm' 0,1/2,z [0,0,w] \( 1/2,0,z [0,0,w] \) \( 1/2,0,\bar{z} [0,0,w] \) \( 0,1/2,\bar{z} [0,0,w] \)

8 e 4.. 0,0,z [0,0,w] \( 1/2,1/2,\bar{z} [0,0,w] \) \( 0,0,\bar{z} [0,0,w] \) \( 1/2,1/2,\bar{z} [0,0,w] \)

4 d m.m'm' 0,1/2,0 [0,0,w] \( 1/2,0,0 [0,0,w] \)

4 c m'.m'm' 0,1/2,1/2 [0,0,0] \( 1/2,0,1/2 [0,0,0] \)

4 b 4/m'.. 0,0,1/2 [0,0,0] \( 1/2,1/2,1/2 [0,0,0] \)

4 a 4/m.. 0,0,0 [0,0,w] \( 1/2,1/2,0 [0,0,w] \)

Symmetry of Special Projections

Along [0,0,1] p4gm1' \( a^* = a \) \( b^* = b \) \( a^* = -c \) \( b^* = b/2 \) \( a^* = -c \) \( b^* = (-a + b)/2 \)
Origin at 0,0,z \ Origin at 0,1/2 \ Origin at x,0,1/2

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Origin at center (4/m) at 4/m1n

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4} \]

Symmetry Operations

(1) \( \bar{1} \) (0,0,0)

(2) \( 2 \) \( 0,0,z \) \( (2z,0,0,0) \)

(3) \( 4 \) \( 0,0,z \) \( (4z,0,0,0) \)

(4) \( 4 \) \( 0,0,z \) \( (4z^{-1},0,0,0) \)

(5) \( 2 \) \( (0,1/2,0,0) \) \( 1/4,y,1/4 \)

(6) \( 2 \) \( (1/2,0,0,0) \) \( x,1/4,1/4 \)

(7) \( 4 \) \( (1/2,1/2,0,0) \) \( x,x,1/4 \)

(8) \( 2 \) \( x,x+1/2,1/4 \)

(10) \( m \) \( x,y,0 \) \( (m_x,0,0,0) \)

(11) \( 4 \) \( 0,0,z;0,0,0 \) \( (4z,0,0,0) \)

(12) \( 4 \) \( 0,0,z;0,0,0 \) \( (4z^{-1},0,0,0) \)

(9) \( \bar{1} \) \( 0,0,0 \)

(10) \( m \) \( x,y,0 \) \( (m_x,0,0,0) \)

(11) \( 4 \) \( 0,0,z;0,0,0 \) \( (4z,0,0,0) \)

(12) \( 4 \) \( 0,0,z;0,0,0 \) \( (4z^{-1},0,0,0) \)

(13) \( n \) \( (1/2,0,1/2) \) \( x,1/4,z \)

(14) \( n \) \( (0,1/2,1/2) \) \( 1/4,y,z \)

(15) \( c \) \( (0,0,1/2) \) \( x+1/2,y,z \)

(16) \( n \) \( (1/2,1/2,1/2) \) \( x,x,z \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>i</td>
<td>1 (1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x̅,y̅,z [u̅,v̅,w̅]</td>
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<tr>
<td></td>
<td></td>
<td>(3) y̅,x̅,z [v̅,u̅,w̅]</td>
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<td></td>
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<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(7) y̅+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>8</td>
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<td>m.. x,y,0 [0,0,w]</td>
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<tr>
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<td>c</td>
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<tr>
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<td>a</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Symmetry</th>
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<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4gm1'</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>c_\perp 2mm'</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p_{2\perp} 2m'm'</td>
</tr>
</tbody>
</table>

Origin at 0,0,0
Origin at center (4/m1') at 4/m1n1'

Asymmetric unit  \(0 \leq x \leq 1/2;\quad 0 \leq y \leq 1/2;\quad 0 \leq z \leq 1/4\)

Symmetry Operations

For 1 + set

1. \(1\) at \((0,0,0)\)
2. \((12)\) \(0,0,z\) \(0,0,0\)
3. \((13)\) \(0,0,0\) \(0,0,0\)
4. \((14)\) \(0,0,0\) \(0,0,0\)
5. \((15)\) \(0,0,0\) \(0,0,0\)
6. \((16)\) \(0,0,0\) \(0,0,0\)
7. \((17)\) \(0,0,0\) \(0,0,0\)
8. \((18)\) \(0,0,0\) \(0,0,0\)
9. \((19)\) \(0,0,0\) \(0,0,0\)
10. \((20)\) \(0,0,0\) \(0,0,0\)
11. \((21)\) \(0,0,0\) \(0,0,0\)
12. \((22)\) \(0,0,0\) \(0,0,0\)
13. \((23)\) \(0,0,0\) \(0,0,0\)
14. \((24)\) \(0,0,0\) \(0,0,0\)
15. \((25)\) \(0,0,0\) \(0,0,0\)
16. \((26)\) \(0,0,0\) \(0,0,0\)
For 1' + set

<table>
<thead>
<tr>
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<th>Coordinates</th>
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<tr>
<td>16 i 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) (\overline{x},\overline{y},\overline{z}) [0,0,0]</td>
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<tr>
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<td>(3) (y,\overline{x},\overline{z}) [0,0,0]</td>
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<td>(4) (x,\overline{y},\overline{z}) [0,0,0]</td>
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<td></td>
<td>(5) (\overline{x}+1/2,y+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(6) (x+1/2,\overline{y}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(7) (y+1/2,\overline{x}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(8) (\overline{y}+1/2,\overline{x}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(9) (\overline{x},\overline{y},\overline{z}) [0,0,0]</td>
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<td></td>
<td>(10) (x,y,\overline{z}) [0,0,0]</td>
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<tr>
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<td>(11) (y,\overline{x},\overline{z}) [0,0,0]</td>
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<tr>
<td></td>
<td>(12) (\overline{y},x,\overline{z}) [0,0,0]</td>
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<tr>
<td></td>
<td>(13) (x+1/2,\overline{y}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(14) (\overline{x}+1/2,\overline{y}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(15) (\overline{y}+1/2,\overline{x}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(16) (y+1/2,\overline{x}+1/2,\overline{z}+1/2) [0,0,0]</td>
</tr>
<tr>
<td>8 h m..1'</td>
<td>x,y,0 [0,0,0]</td>
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<td></td>
<td>(\overline{x},\overline{y},\overline{z}) [0,0,0]</td>
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<tr>
<td></td>
<td>(y,\overline{x},\overline{z}) [0,0,0]</td>
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<td>(x,\overline{y},\overline{z}) [0,0,0]</td>
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<td>(\overline{x}+1/2,y+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(x+1/2,\overline{y}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(y+1/2,\overline{x}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<td>(\overline{y}+1/2,\overline{x}+1/2,\overline{z}+1/2) [0,0,0]</td>
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<tr>
<td>8 g .21'</td>
<td>x,x+1/2,1/4 [0,0,0]</td>
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<td>(\overline{x},\overline{x}+1/2,1/4) [0,0,0]</td>
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<td>(\overline{y},x+1/2,1/4) [0,0,0]</td>
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<td>(\overline{x}+1/2,\overline{x},1/4) [0,0,0]</td>
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<td>(\overline{x},\overline{x}+1/2,3/4) [0,0,0]</td>
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<td>(\overline{x},x+1/2,3/4) [0,0,0]</td>
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<td>(x+1/2,\overline{x},3/4) [0,0,0]</td>
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<td>(\overline{x}+1/2,\overline{x},3/4) [0,0,0]</td>
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<tr>
<td>8 f 2..1'</td>
<td>0,1/2,z [0,0,0]</td>
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<td>(1/2,z+1/2) [0,0,0]</td>
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<td>(1/2,z+1/2) [0,0,0]</td>
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<td>(1/2,z+1/2) [0,0,0]</td>
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<tr>
<td>4 e 4..1'</td>
<td>0,0,z [0,0,0]</td>
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<tr>
<td></td>
<td>(1/2,1/2,z+1/2) [0,0,0]</td>
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<td>(1/2,1/2,z+1/2) [0,0,0]</td>
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<tr>
<td>4 d 2.221'</td>
<td>0,1/2,1/4 [0,0,0]</td>
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<td>(1/2,0,1/4) [0,0,0]</td>
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<td>(1/2,3/4) [0,0,0]</td>
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<td>(1/2,0,3/4) [0,0,0]</td>
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<tr>
<td>4 c 2/m..1'</td>
<td>0,1/2,0 [0,0,0]</td>
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<td>(1/2,0,1/2) [0,0,0]</td>
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<td>(1/2,0,1/2) [0,0,0]</td>
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<td>(1/2,0,1/2) [0,0,0]</td>
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</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.
2  b  4/m..1’  0,0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]
2  a  4/m..1’  0,0,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4gm1’</th>
<th>Along [1,0,0]</th>
<th>c 2mm1’</th>
<th>Along [1,1,0]</th>
<th>p 2mm1’</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
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<td>Origin at x,x,0</td>
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</tbody>
</table>

Continued 128.2.1067 P4/mnc1’
**Origin** at center (4/m'') at 4/m'1n

**Asymmetric unit**

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

**Symmetry Operations**

1. 1
   (1|0,0,0)

2. 2  0,0,z
   (2z|0,0,0)

3. 4+ 0,0,z
   (4z|0,0,0)

4. 4- 0,0,z
   (4z|0,0,0)

5. 2' (0,1/2,0) 1/4,y,1/4
   (2y|1/2,1/2,1/2')

6. 2' (1/2,0,0) x,1/4,1/4
   (2x|1/2,1/2,1/2')

7. 2' (1/2,1/2,0) x,x,1/4
   (2xy|1/2,1/2,1/2')

8. 2' x,x+1/2,1/4
   (2xy|1/2,1/2,1/2')

9. m
   (1|0,0,0)

10. m' x,y,0
    (mz|0,0,0')

11. m+ 0,0,z; 0,0,0
    (4z|0,0,0')

12. m- 0,0,z; 0,0,0
    (4z|0,0,0')

13. n (1/2,0,1/2) x,1/4,z
    (m|1/2,1/2,1/2)

14. n (0,1/2,1/2) 1/4,y,z
    (m|1/2,1/2,1/2)

15. c (0,0,1/2) x+1/2,z
    (mxy|1/2,1/2,1/2)

16. n (1/2,1/2,1/2) x,x,z
    (m|1/2,1/2,1/2)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>16</td>
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<tr>
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<td>(3)</td>
<td>y̅,x,z [v̅,u̅,w]</td>
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<td>(4)</td>
<td>y,x̅,z [v̅,u̅,w]</td>
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<td>(5)</td>
<td>x̅+1/2,y+1/2,z+1/2 [u̅,v̅,w]</td>
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<td>8</td>
<td>h</td>
<td>m'..</td>
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<td>y̅,x̅,0 [v̅,u̅,0]</td>
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<td>y+1/2,x+1/2,z+1/2 [v̅,u̅,w]</td>
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<td>..2'</td>
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<tr>
<td>(6)</td>
<td>x̅+1/2,x̅+1/2,3/4 [u̅,u̅,w]</td>
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<tr>
<td>8</td>
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<td>2..</td>
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<tr>
<td>(1)</td>
<td>1/2,0,z [0,0,w]</td>
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<tr>
<td>4</td>
<td>d</td>
<td>2.2'2'</td>
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<td>1/2,0,0 [0,0,0]</td>
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<tr>
<td>2</td>
<td>b</td>
<td>4/m'..</td>
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<tr>
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<td>1/2,1/2,0 [0,0,0]</td>
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<td>(2)</td>
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<tr>
<td>2</td>
<td>a</td>
<td>4/m'..</td>
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<td>0,0,0 [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4gm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>c_p 2m'm'</th>
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</thead>
<tbody>
<tr>
<td>a^* = b</td>
<td>b^* = c</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p_2c 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = -c/2</td>
<td>b^* = (-a + b)/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,0,0

128.3.1068 - 2 - 2194
Origin at center (4/m) at 4/m1n

Asymmetric unit  
\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}\]

Symmetry Operations

1. \([1, 0, 0, 0]\)
2. \([2, 0, 0, z, (2_z, 0, 0, 0)]\)
3. \([4^+, 0, 0, z, (4_z, 0, 0, 0')]\)
4. \([4^- 0, 0, z, (4_z^{-1}, 0, 0, 0)']\)
5. \([2', (0, 1/2, 0), 1/4, y, 1/4, (2_y, 1/2, 1/2, 1/2)']\)
6. \([2', (1/2, 0, 0), x, 1/4, 1/4, (2_x, 1/2, 1/2, 1/2)']\)
7. \([2 (1/2, 1/2, 0), x, x, 1/4, (2_y, 1/2, 1/2, 1/2)']\)
8. \([2, x, x+1/2, 1/4, (2_y, 1/2, 1/2, 1/2)']\)
9. \([\overline{1}, 0, 0, 0]\)
10. \([m, x, y, 0, (m_x, 0, 0, 0)]\)
11. \([\overline{4}^+, 0, 0, z, 0, 0, 0, (\overline{4}_z, 0, 0, 0)']\)
12. \([\overline{4}^-, 0, 0, z, 0, 0, 0, (\overline{4}_z^{-1}, 0, 0, 0)']\)
13. \([n', (1/2, 0, 1/2), x, 1/4, z, (m_y, 1/2, 1/2, 1/2)']\)
14. \([n', (0, 1/2, 1/2), 1/4, y, z, (m_y, 1/2, 1/2, 1/2)']\)
15. \([c (0, 0, 1/2), x+1/2, x, z, (m_x, 1/2, 1/2, 1/2)]\)
16. \([n (1/2, 1/2, 1/2), x, x, z, (m_x, 1/2, 1/2, 1/2)]\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
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<tr>
<td>16</td>
<td>i</td>
<td>1 (1) x,y,z [u,v,w]</td>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z [v,u,w]</td>
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<td>(4) y,x,z [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(13) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(14) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(15) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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</tbody>
</table>

| 8            | h              | m.. x,y,0 [0,0,w] |
|              |                | x,y,0 [0,0,w] |
|              |                | y,x,0 [0,0,w] |
|              |                | y,x,0 [0,0,w] |
|              |                | x+1/2,y+1/2,z+1/2 [0,0,w] |
|              |                | y+1/2,x+1/2,z+1/2 [0,0,w] |
|              |                | y+1/2,x+1/2,z+1/2 [0,0,w] |

| 8            | g              | ..2 x+1/2,1/4 [u,u,0] |
|              |                | x+1/2,1/4 [u,u,0] |
|              |                | x+1/2,1/4 [u,u,0] |
|              |                | x+1/2,1/4 [u,u,0] |
|              |                | x+1/2,1/4 [u,u,0] |
|              |                | x+1/2,1/4 [u,u,0] |
|              |                | x+1/2,1/4 [u,u,0] |

| 8            | f              | 2.. 0,1/2,z [0,0,w] |
|              |                | 0,1/2,z [0,0,w] |
|              |                | 0,1/2,z [0,0,w] |
|              |                | 0,1/2,z [0,0,w] |
|              |                | 0,1/2,z [0,0,w] |
|              |                | 0,1/2,z [0,0,w] |
|              |                | 0,1/2,z [0,0,w] |

| 4            | e              | 4'.. 0,0,z [0,0,0] |
|              |                | 0,0,z [0,0,0] |
|              |                | 0,0,z [0,0,0] |
|              |                | 0,0,z [0,0,0] |
|              |                | 0,0,z [0,0,0] |
|              |                | 0,0,z [0,0,0] |
|              |                | 0,0,z [0,0,0] |

| 4            | d              | 2.22 0,1/2,1/4 [0,0,0] |
|              |                | 0,1/2,1/4 [0,0,0] |
|              |                | 0,1/2,1/4 [0,0,0] |
|              |                | 0,1/2,1/4 [0,0,0] |
|              |                | 0,1/2,1/4 [0,0,0] |
|              |                | 0,1/2,1/4 [0,0,0] |
|              |                | 0,1/2,1/4 [0,0,0] |

| 4            | c              | 2/m.. 0,1/2,0 [0,0,w] |
|              |                | 0,1/2,0 [0,0,w] |
|              |                | 0,1/2,0 [0,0,w] |
|              |                | 0,1/2,0 [0,0,w] |
|              |                | 0,1/2,0 [0,0,w] |
|              |                | 0,1/2,0 [0,0,w] |
|              |                | 0,1/2,0 [0,0,w] |

| 2            | b              | 4'/m.. 0,0,1/2 [0,0,0] |
|              |                | 0,0,1/2 [0,0,0] |
|              |                | 0,0,1/2 [0,0,0] |
|              |                | 0,0,1/2 [0,0,0] |
|              |                | 0,0,1/2 [0,0,0] |
|              |                | 0,0,1/2 [0,0,0] |
|              |                | 0,0,1/2 [0,0,0] |

| 2            | a              | 4'/m.. 0,0,0 [0,0,0] |
|              |                | 0,0,0 [0,0,0] |
|              |                | 0,0,0 [0,0,0] |
|              |                | 0,0,0 [0,0,0] |
|              |                | 0,0,0 [0,0,0] |
|              |                | 0,0,0 [0,0,0] |
|              |                | 0,0,0 [0,0,0] |

Symmetry of Special Projections
Along [0,0,1] p4gm1' a* = a  b* = b Origin at 0,0,z
Along [1,0,0] c2mm' a* = -c  b* = b Origin at x,0,0
Along [1,1,0] p2cm 2m'm' a* = -c/2  b* = (-a + b)/2 Origin at x,x,1/4
Along [0,1,0] p2c 2m'm' a* = a  b* = b Origin at 0,0,z
Along [0,0,1] p4gm1' a* = a  b* = b Origin at 0,0,z
Origin at center (4'/m) at 4'/m1n'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

1. 1 (1 0 0)
2. 2 0 0, z (2z 0 0, 0)
3. 4+ 0 0, z (4z 0 0, 0)
4. 4+ 0 0, z (4z-1 0 0, 0)
5. 2 (0, 1/2, 0) 1/4, y, 1/4 (2y 1/2, 1/2, 1/2)
6. 2 (1/2, 0, 0) x, 1/4, 1/4 (2x 1/2, 1/2, 1/2)
7. 2' (1/2, 1/2, 0) x, x, 1/4 (2xy 1/2, 1/2, 1/2)
8. 2' x, x + 1/2, 1/4 (2xy 1/2, 1/2, 1/2)
9. 2 0, 0, 0 (1 0, 0, 0)
10. m x, y, 0 (mz 0, 0, 0)
11. 4- z, 0, 0, 0 (4z 0, 0, 0)
12. 4- z, 0, 0, 0 (4z-1 0, 0, 0)
13. n (1/2, 0, 1/2) x, 1/4, z (m, 1/2, 1/2, 1/2)
14. n (0, 1/2, 1/2) 1/4, y, z (m, 1/2, 1/2, 1/2)
15. c' (0, 0, 1/2) x + 1/2, x, z (m, 1/2, 1/2, 1/2)
16. n' (1/2, 1/2, 1/2) x, x, z (m, 1/2, 1/2, 1/2)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

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</table>

| 8            | h              | m.. x,y,0 [0,0,w] |
|              |                | x̅,y,0 [0,0,w] |
|              |                | y̅,x,0 [0,0,w] |
|              |                | y,x,0 [0,0,w] |
|              |                | x+1/2,y+1/2,1/2 [0,0,w] |
|              |                | x+1/2,y+1/2,1/2 [0,0,w] |
|              |                | y+1/2,x+1/2,1/2 [0,0,w] |
|              |                | y+1/2,x+1/2,1/2 [0,0,w] |

| 8            | g              | ..2' x,x+1/2,1/4 [u,u,w] |
|              |                | x̅,x+1/2,1/4 [u,u,w] |
|              |                | x̅,x+1/2,1/4 [u,u,w] |
|              |                | x+1/2,x+1/2,1/4 [u,u,w] |
|              |                | x+1/2,x+1/2,1/4 [u,u,w] |

| 8            | f              | 2.. 0,1/2,z [0,0,w] |
|              |                | 1/2,0,z [0,0,w] |
|              |                | 1/2,0,z+1/2 [0,0,w] |
|              |                | 1/2,0,z+1/2 [0,0,w] |

| 4            | e              | 4'.. 0,0,z [0,0,0] |
|              |                | 1/2,1/2,z+1/2 [0,0,0] |
|              |                | 0,0,z [0,0,0] |
|              |                | 1/2,1/2,z+1/2 [0,0,0] |

| 4            | d              | 2.2'2' 0,1/2,1/4 [0,0,w] |
|              |                | 1/2,0,1/4 [0,0,w] |
|              |                | 0,1/2,3/4 [0,0,w] |
|              |                | 1/2,0,3/4 [0,0,w] |

| 4            | c              | 2/m.. 0,1/2,0 [0,0,w] |
|              |                | 1/2,0,0 [0,0,w] |
|              |                | 1/2,0,1/2 [0,0,w] |
|              |                | 0,1/2,1/2 [0,0,w] |

| 2            | b              | 4'/m.. 0,1/2 [0,0,0] |
|              |                | 1/2,1,2 [0,0,0] |

| 2            | a              | 4'/m.. 0,0 [0,0,0] |
|              |                | 1/2,1/2,1/2 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p4gm1’

\[ \mathbf{a^*} = \mathbf{a} \quad \mathbf{b^*} = \mathbf{b} \]

Origin at 0,0,z

Along [1,0,0] c\(^{-}&\) 2’mm’

\[ \mathbf{a^*} = -\mathbf{c} \quad \mathbf{b^*} = \mathbf{b} \]

Origin at x,0,0

Along [1,1,0] p 2’m’

\[ \mathbf{a^*} = -\mathbf{c}/2 \quad \mathbf{b^*} = (-\mathbf{a} + \mathbf{b})/2 \]

Origin at x,x,0
Origin at center (4/m'c) at 4/m'1n

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

1. \(1\) \( 0,0,0 \)
2. \(2\) \( 0,0,z \)
\[ (2z | 0,0,0) \]
3. \(4^+\) \( 0,0,z \)
\[ (4z | 0,0,0)' \]
4. \(4^-\) \( 0,0,z \)
\[ (4z^- | 0,0,0)' \]
5. \(2\) \( (0,1/2,0) \)
\[ 1/4,1/4,1/4 \]
\[ (2x | 1/2,1/2,1/2) \]
6. \(2\) \( (1/2,0,0) \)
\[ x,1/4,1/4 \]
\[ (2x_0 | 1/2,1/2,1/2) \]
7. \(2'\) \( (1/2,1/2,0) \)
\[ x,x,1/4 \]
\[ (2x_0 | 1/2,1/2,1/2)' \]
8. \(2'\) \( x,x+1/2,1/4 \)
\[ (2x_0 | 1/2,1/2,1/2)' \]
9. \(\overline{1}\) \( 0,0,0 \)
\[ (1 | 0,0,0)' \]
10. \(m'\) \( x,y,0 \)
\[ (m_2 | 0,0,0)' \]
11. \(\overline{4}^+\) \( 0,0,z; 0,0,0 \)
\[ (4z | 0,0,0) \]
12. \(\overline{4}^-\) \( 0,0,z; 0,0,0 \)
\[ (4z^- | 0,0,0) \]
13. \(n'\) \( (1/2,0,1/2) \)
\[ x,1/4,z \]
\[ (m_2 | 1/2,1/2,1/2)' \]
14. \(n'\) \( (0,1/2,1/2) \)
\[ 1/4,y,z \]
\[ (m_2 | 1/2,1/2,1/2)' \]
15. \(c\) \( (0,0,1/2) \)
\[ x+1/2,x,z \]
\[ (m_2 | 1/2,1/2,1/2) \]
16. \(n\) \( (1/2,1/2,1/2) \)
\[ x,x,z \]
\[ (m_2 | 1/2,1/2,1/2) \]
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 i 1 (1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(9) x,y,z [u,v,w]</td>
<td>(10) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(11) y,x,z [v,u,w]</td>
<td>(12) y,x,z [v,u,w]</td>
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<tr>
<td>(13) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(14) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td>(15) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>8 h m’..</th>
<th>x,y,0 [u,v,0]</th>
<th>x,y,0 [u,v,0]</th>
<th>y,x,0 [v,u,0]</th>
<th>y,x,0 [v,u,0]</th>
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<tr>
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<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<table>
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<tr>
<th>8 g ..2’</th>
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<th>x+1/2,1/4 [u,u,w]</th>
<th>x+1/2,1/4 [u,u,w]</th>
<th>x+1/2,1/4 [u,u,w]</th>
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<tbody>
<tr>
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<td>x+1/2,3/4 [u,u,w]</td>
<td>x+1/2,3/4 [u,u,w]</td>
<td>x+1/2,3/4 [u,u,w]</td>
<td>x+1/2,3/4 [u,u,w]</td>
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</tbody>
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<thead>
<tr>
<th>8 f 2..</th>
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<th>1/2,0,z [0,0,w]</th>
<th>1/2,0,z [0,0,w]</th>
<th>1/2,0,z [0,0,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>4 e 4’..</th>
<th>0,0,z [0,0,0]</th>
<th>1/2,1/2,z+1/2 [0,0,0]</th>
<th>0,0,z [0,0,0]</th>
<th>1/2,1/2,z+1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 2.2’</td>
<td>1/2,0,1/4 [0,0,w]</td>
<td>1/2,0,1/4 [0,0,w]</td>
<td>1/2,3/4 [0,0,w]</td>
<td>1/2,3/4 [0,0,w]</td>
</tr>
<tr>
<td>4 c 2/m’..</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2 b 4’/m’..</th>
<th>0,0,1/2 [0,0,0]</th>
<th>1/2,1/2,0 [0,0,0]</th>
<th>0,0,1/2 [0,0,0]</th>
<th>1/2,1/2,0 [0,0,0]</th>
</tr>
</thead>
<tbody>
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<td>2 a 4’/m’..</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4’g’m

- \(a^* = a\)
- \(b^* = b\)

Origin at 0,0,z

Along [1,0,0] c 2m’m’

- \(a^* = a\)
- \(b^* = c\)

Origin at x,0,0

Along [1,1,0] \(p_{2a} \cdot 2m’m’\)

- \(a^* = -c/2\)
- \(b^* = (-a + b)/2\)

Origin at x,x,0

128.6.1071 - 2 - 2200
Origin at center (4/m) at 4/m1n'

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4} \]

Symmetry Operations

1. \( 1 \) 
   \( (1|0,0,0) \)
2. \( 2 \) \( 0,0,z \)
   \( (2_z|0,0,0) \)
3. \( 4^+ \) \( 0,0,z \)
   \( (4_z|0,0,0) \)
4. \( 4^- \) \( 0,0,z \)
   \( (4_z^{-1}|0,0,0) \)
5. \( 2' \) (0,1/2,0) \( 1/4, y, 1/4 \)
   \( (2_x|1/2,1/2,1/2)' \)
6. \( 2' \) (1/2,0,0) \( x, 1/4, 1/4 \)
   \( (2_x|1/2,1/2,1/2)' \)
7. \( 2' \) (1/2,1/2,0) \( x, x, 1/4 \)
   \( (2_x|x,1/4,1/4) \)
8. \( 2' \) \( x, x + 1/2, 1/4 \)
   \( (2_x|x,1/4,1/4) \)
9. \( \bar{1} \) \( 0,0,0 \)
   \( (1|0,0,0) \)
10. \( m \) \( x, y, 0 \)
    \( (m_x|0,0,0) \)
11. \( \bar{4}^+ \) \( 0,0,z; 0,0,0 \)
    \( (\bar{4}_z|0,0,0) \)
12. \( \bar{4}^- \) \( 0,0,z; 0,0,0 \)
    \( (\bar{4}_z^{-1}|0,0,0) \)
13. \( n' \) (1/2,0,1/2) \( x, 1/4, z \)
    \( (m_y|1/2,1/2,1/2)' \)
14. \( n' \) (0,1/2,1/2) \( 1/4, y, z \)
    \( (m_x|1/2,1/2,1/2)' \)
15. \( c' \) (0,0,1/2) \( x+1/2, x, z \)
    \( (m_{xy}|1/2,1/2,1/2)' \)
16. \( n' \) (1/2,1/2,1/2) \( x, x, z \)
    \( (m_{xy}|1/2,1/2,1/2)' \)
Continued

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>i</td>
<td>1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) y,x,z [v,u,w] (4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) x+1/2,y+1/2,z+1/2 [u,v,w] (6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w] (8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(9) x,y,z [v,u,w] (10) x,y,z [v,u,w]</td>
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<td></td>
<td>(11) y,x,z [v,u,w] (12) y,x,z [v,u,w]</td>
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<td></td>
<td></td>
<td></td>
<td>(13) y+1/2,x+1/2,z+1/2 [v,u,w] (14) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(15) y+1/2,x+1/2,z+1/2 [v,u,w] (16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>h</td>
<td>m..</td>
<td>x,y,0 [0,0,w] x,y,0 [0,0,w] y,x,0 [0,0,w] y,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x+1/2,y+1/2,z+1/2 [0,0,w] x+1/2,y+1/2,z+1/2 [0,0,w] y+1/2,x+1/2,z+1/2 [0,0,w] y+1/2,x+1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
<td>..2’</td>
<td>x,x+1/2,1/4 [u,u,w] x,x+1/2,1/4 [u,u,w] x,x+1/2,1/4 [u,u,w] x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x,x+1/2,3/4 [u,u,w] x,x+1/2,3/4 [u,u,w] x,x+1/2,3/4 [u,u,w] x,x+1/2,3/4 [u,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>2..</td>
<td>0,1/2,z [0,0,w] 1/2,0,z [0,0,w] 1/2,0,z [0,0,w] 0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>4..</td>
<td>0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 0,0,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>2.2’2’</td>
<td>0,1/2,1/4 [0,0,w] 1/2,0,1/4 [0,0,w] 1/2,0,1/4 [0,0,w] 1/2,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>2/m..</td>
<td>0,1/2,0 [0,0,w] 1/2,0,0 [0,0,w] 1/2,0,0 [0,0,w] 1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4/m..</td>
<td>0,0,1/2 [0,0,w] 1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4/m..</td>
<td>0,0,0 [0,0,w] 1/2,1/2,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4gm1’

\[
\begin{align*}
\mathbf{a}^* &= \mathbf{a} & \mathbf{b}^* &= \mathbf{b} \\
\text{Origin at } 0,0,z
\end{align*}
\]

Along [1,0,0] c 2’mm’

\[
\begin{align*}
\mathbf{a}^* &= -\mathbf{c} & \mathbf{b}^* &= \mathbf{b} \\
\text{Origin at } x,0,0
\end{align*}
\]

Along [1,1,0] p 2’mm’

\[
\begin{align*}
\mathbf{a}^* &= -\mathbf{c}/2 & \mathbf{b}^* &= (-\mathbf{a} + \mathbf{b})/2 \\
\text{Origin at } x,x,0
\end{align*}
\]
Origin at center ($4'/m'$) at $4'/m'1n'$

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/4$

Symmetry Operations

1. 1
2. $2' \ 0,0,z$
3. $4^{+} \ 0,0,z$
4. $4^{-} \ 0,0,z$
5. $2' \ (0,1/2,0) \ 1/4,y,1/4$
6. $2' \ (1/2,0,0) \ x,1/4,1/4$
7. $2 \ (1/2,1/2,0) \ x,x,1/4$
8. $2 \ x,x+1/2,1/4$
9. $\overline{1} \ 0,0,0$
10. $m' \ x,y,0$
11. $\overline{4}^{-} \ 0,0,z \; 0,0,0$
12. $\overline{4}^{-} \ 0,0,z \; 0,0,0$
13. $n \ (1/2,0,1/2) \ x,1/4,z$
14. $n \ (0,1/2,1/2) \ 1/4,y,z$
15. $c' \ (0,0,1/2) \ x+1/2,x,z$
16. $n' \ (1/2,1/2,1/2) \ x,x,z$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

| Positions |  |  |
|-----------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| Multiplicity, Wyckoff letter, Site Symmetry. | Coordinates |  |
| 16 | i | 1 | (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] |
| | | | (3) y,x,z [v,u,w] | (4) y,x,z [v,u,w] |
| | | | (5) x+1/2,y+1/2,z+1/2 [u,v,w] | (6) x+1/2,y+1/2,z+1/2 [u,v,w] |
| | | | (7) y+1/2,x+1/2,z+1/2 [v,u,w] | (8) y+1/2,x+1/2,z+1/2 [v,u,w] |
| | | | (9) x,y,z [u,v,w] | (10) x,y,z [u,v,w] |
| | | | (11) y,x,z [v,u,w] | (12) y,x,z [v,u,w] |
| | | | (13) x+1/2,y+1/2,z+1/2 [u,v,w] | (14) x+1/2,y+1/2,z+1/2 [u,v,w] |
| | | | (15) y+1/2,x+1/2,z+1/2 [v,u,w] | (16) y+1/2,x+1/2,z+1/2 [v,u,w] |
| 8 | h | m'.. | x,y,0 [u,v,0] | x,y,0 [u,v,0] |
| | | | y,z,0 [v,u,0] | y,z,0 [v,u,0] |
| | | | (x+1/2,y+1/2,z+1/2 [u,v,w]) | (y+1/2,x+1/2,z+1/2 [v,u,w]) |
| | | | (x+1/2,y+1/2,z+1/2 [u,v,w]) | (y+1/2,x+1/2,z+1/2 [v,u,w]) |
| 8 | g | .2 | x,x+1/2,1/4 [u,u,0] | x,x+1/2,1/4 [u,u,0] |
| | | | x,y,1/2,z [0,0,w] | x,y,1/2,z [0,0,w] |
| | | | (x+1/2,y+1/2,z+1/2 [u,v,w]) | (y+1/2,x+1/2,z+1/2 [v,u,w]) |
| | | | (x+1/2,y+1/2,z+1/2 [u,v,w]) | (y+1/2,x+1/2,z+1/2 [v,u,w]) |
| | 8 | 2.. | 0,1/2,z [0,0,w] | 1/2,0,z [0,0,w] |
| | | | 1/2,0,z [0,0,w] | 1/2,0,z [0,0,w] |
| | | | 0,1/2,z+1/2 [0,0,0] | 0,1/2,z+1/2 [0,0,0] |
| | | | 0,1/2,z+1/2 [0,0,0] | 0,1/2,z+1/2 [0,0,0] |
| 4 | e | 4'.. | 0,0,z [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] |
| | | | 0,0,z [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] |
| 4 | d | 2.22 | 0,1/2,1/4 [0,0,0] | 1/2,0,1/4 [0,0,0] |
| | | | 0,1/2,1/4 [0,0,0] | 1/2,0,1/4 [0,0,0] |
| 4 | c | 2/m'.. | 0,1/2,0 [0,0,0] | 1/2,0,0 [0,0,0] |
| | | | 0,1/2,0 [0,0,0] | 1/2,0,0 [0,0,0] |
| 2 | b | 4'/m'.. | 0,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| | | | 0,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 2 | a | 4'/m'.. | 0,0,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

Symmetry of Special Projections

- Along [0,0,1] p4'gm'
  \[ a^* = a \quad b^* = b \]
  Origin at 0,0,z

- Along [1,0,0] c_{p\prime} 2m'm'
  \[ a^* = b \quad b^* = c \]
  Origin at x,0,0

- Along [1,1,0] p 2m'm'
  \[ a^* = (-a + b)/2 \quad b^* = c/2 \]
  Origin at x,x,0
Origin at center (4/m' ) at 4/m'1n'

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

(1) \[ 1 \]
(1' \[ 0,0,0 \])

(5) \[ 2 \]
(0,1/2,0) \[ 1/4,y,1/4 \]
(2 \[ 1/2,1/2,1/2 \])

(9) \[ \bar{1} \]
0,0,0
(1' \[ 0,0,0 \])

(13) \[ \bar{n}' \]
(1/2,0,1/2) \[ x,1/4,z \]
(m \[ 1/2,1/2,1/2 \])

(14) \[ \bar{n}' \]
(0,1/2,1/2) \[ 1/4,y,z \]
(m \[ 1/2,1/2,1/2 \])

(15) \[ c' \]
(0,0,1/2) \[ x+1/2,x,z \]
(m \[ 1/2,1/2,1/2 \])

(16) \[ n' \]
(1/2,1/2,1/2) \[ x,x,z \]
(m \[ 1/2,1/2,1/2 \])

\[ (1) \quad 1 \]
\[ (2) \quad 2 \]
[0,0,z]
\[ (2_x,0,0,0) \]

\[ (3) \quad 4^+ \]
[0,0,z]
\[ (4_z,0,0,0) \]

\[ (4) \quad 4^- \]
[0,0,z]
\[ (4_z^{-1},0,0,0) \]

\[ (5) \quad 2 \]
(0,1/2,0) \[ 1/4,y,1/4 \]
(2 \[ 1/2,1/2,1/2 \])

\[ (6) \quad 2 \]
(1/2,0,0) \[ x,1/4,1/4 \]
(2 \[ 1/2,1/2,1/2 \])

\[ (7) \quad 2 \]
(1/2,1/2,0) \[ x,x,1/4 \]
(2 \[ 1/2,1/2,1/2 \])

\[ (8) \quad 2 \]
x,x+1/2,1/4
(2 \[ 1/2,1/2,1/2 \])

\[ (9) \quad \bar{1} \]
0,0,0
(1' \[ 0,0,0 \])

\[ (10) \quad m' \]
x,y,0
(m \[ 0,0,0 \])

\[ (11) \quad \bar{4}^+ \]
0,0,z; 0,0,0
(4 \[ 0,0,0 \])

\[ (12) \quad \bar{4}^- \]
0,0,z; 0,0,0
(4 \[ 0,0,0 \])

\[ (13) \quad \bar{n}' \]
(1/2,0,1/2) \[ x,1/4,z \]
(m \[ 1/2,1/2,1/2 \])

\[ (14) \quad \bar{n}' \]
(0,1/2,1/2) \[ 1/4,y,z \]
(m \[ 1/2,1/2,1/2 \])

\[ (15) \quad c' \]
(0,0,1/2) \[ x+1/2,x,z \]
(m \[ 1/2,1/2,1/2 \])

\[ (16) \quad n' \]
(1/2,1/2,1/2) \[ x,x,z \]
(m \[ 1/2,1/2,1/2 \])
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>i</td>
<td>1</td>
</tr>
<tr>
<td>8</td>
<td>h</td>
<td>m'</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
<td>..2</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>2..</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>4..</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>2.22</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>2/m'..</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4/m'..</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4/m'..</td>
</tr>
</tbody>
</table>

Coordinates

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) y,x,z [v,u,w]
(4) y,x,z [v,u,w]
(5) x+1/2,y+1/2,z+1/2 [u,v,w]
(6) x+1/2,y+1/2,z+1/2 [u,v,w]
(7) y+1/2,x+1/2,z+1/2 [v,u,w]
(8) y+1/2,x+1/2,z+1/2 [v,u,w]
(9) x,y,z [u,v,w]
(10) x,y,z [u,v,w]
(11) y,x,z [v,u,w]
(12) y,x,z [v,u,w]
(13) x+1/2,y+1/2,z+1/2 [u,v,w]
(14) x+1/2,y+1/2,z+1/2 [u,v,w]
(15) y+1/2,x+1/2,z+1/2 [v,u,w]
(16) y+1/2,x+1/2,z+1/2 [v,u,w]

Symmetry of Special Projections

Along [0,0,1] p4g'm'

a* = a  b* = b

Origin at 0,0,z
Origin at center $\overline{4}m2$ at $\overline{4}/nm2/g$, at $-1/4,1/4,0$ from center (2/m)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

Symmetry Operations

(1) $1$

(2) $2 \begin{pmatrix} 0,0,z \\ 2z,0,0,0 \end{pmatrix}$

(3) $4^+ \begin{pmatrix} 0,1/2,z \\ 4z,1/2,1/2,0 \end{pmatrix}$

(4) $4^- \begin{pmatrix} 1/2,0,z \\ 4z^{-1},1/2,1/2,0 \end{pmatrix}$

(5) $2 \begin{pmatrix} 0,1/2,0 \\ 2,1/2,1/2,0 \end{pmatrix}$

(6) $2 \begin{pmatrix} 1/2,0,0 \\ 2,1/2,1/2,0 \end{pmatrix}$

(7) $2 \begin{pmatrix} x,0,0 \\ 2xy,0,0 \end{pmatrix}$

(8) $2 \begin{pmatrix} x,0,0 \\ 2xy,0,0 \end{pmatrix}$

(9) $\overline{1} \begin{pmatrix} 1/4,1/4,0 \\ 1,1/2,1/2,0 \end{pmatrix}$

(10) $n \begin{pmatrix} 1/2,1/2,0 \\ mz,1/2,1/2,0 \end{pmatrix}$

(11) $\overline{4}^+ \begin{pmatrix} 0,0,z \\ 4z,0,0 \end{pmatrix}$

(12) $\overline{4}^- \begin{pmatrix} 0,0,z; 0,0,0 \\ 4z^{-1},0,0 \end{pmatrix}$

(13) $m \begin{pmatrix} x,0,z \\ mz,0,0,0 \end{pmatrix}$

(14) $m \begin{pmatrix} 0,y,z \\ my,0,0 \end{pmatrix}$

(15) $m \begin{pmatrix} x+1/2,0,0 \\ mx,1/2,1/2,0 \end{pmatrix}$

(16) $g \begin{pmatrix} 1/2,1/2,0 \\ x,x,z \end{pmatrix}$

(mz,1/2,1/2,0)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>x,y,z [u,v,w]</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>4mm</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>j..m</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>i..m</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>h..2</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>g..2</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>f2mm</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>e..2/m</td>
<td></td>
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<tr>
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<td>d..2/m</td>
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</tr>
<tr>
<td>2</td>
<td>c4mm</td>
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</tr>
<tr>
<td>2</td>
<td>b4mm2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a4mm2</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along \([0,0,1]\) \(p_{4\text{mm}}\)

- \(a^* = (a - b)/2\) = \(\mathbf{b}\) = \(\mathbf{c}\)

Origin at \(0,1/2,z\)

Along \([1,0,0]\) \(p2'm'g\)

- \(a^* = (a + b)/2\)

Origin at \([1,0,0]\)

Along \([1,1,0]\) \(p2mm1'\)

- \(a^* = -(a + b)/2\) = \(\mathbf{b}\) = \(\mathbf{c}\)

Origin at \([1,0,0]\)
Origin at center $\overline{4}m21''$ at $\overline{4}/nm2/1''$, at $-1/4,1/4,0$ from center (2/m1'')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x \]

Symmetry Operations

For 1 + set

(1) 1
(1 | 0,0,0)

(5) 2 (0,1/2,0) 1/4,y,0
(2 | 1/2,1/2,0)

(9) $\overline{1}$ 1/4,1/4,0
($\overline{1}$ | 1/2,1/2,0)

(13) m x,0,z
(m | 0,0,0)

(2) 2 0,0,z
(2z | 0,0,0)

(6) 2 (1/2,0,0) x,1/4,0
(2z | 1/2,1/2,0)

(10) n (1/2,1/2,0) x,y,0
(mz | 1/2,1/2,0)

(14) m 0,y,z
(mz | 0,0,0)

(3) 4' 0,1/2,z
(4z | 1/2,1/2,0)

(7) 2 x,x,0
(2y | 0,0,0)

(11) $\overline{4}'$ 0,0,z; 0,0,0
($\overline{4}z$ | 0,0,0)

(15) m x+1/2,x,z
(mxy | 1/2,1/2,0)

(4) 4' 1/2,0,z
(4z | 1/2,1/2,0)

(8) 2 x,x,0
(2y | 0,0,0)

(12) $\overline{4}'$ 0,0,z; 0,0,0
($\overline{4}z$ | 0,0,0)

(16) g (1/2,1/2,0) x,x,z
(mxy | 1/2,1/2,0)
Continued

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P4/nmm1'

For 1' + set

(1) 1'  
(1 0,0,0)'  
(2) 2' 0,0,z  
(2 0,0,0)'  
(3) 4' 0,1/2,z  
(4 1/2,1/2,0)'  
(4 1/2,0,0)'  
(4 -1 1/2,1/2,0)'

(5) 2'(0,1/2,0) 1/4,y,0  
(2 1/2,1/2,0)'  
(6) 2'(1/2,0,0) x,1/4,0  
(2 0,0,0)'  
(7) 2' x,x,0  
(2 z 0,0,0)'  
(8) 2' x,x,0  
(2 z 0,0,0)'

(9) 1' 1/4,1/4,0  
(1 2/1,1/2,0)'  
(10) n' (1/2,1/2,0) y,0,z  
(1 0,0,0)'  
(11) 4' 0,0,z; 0,0,0  
(4 0,0,0)'  
(12) 4' 0,0,z; 0,0,0  
(4 0,0,0)'

(13) m' x,0,z  
(1 0,0,0)'  
(14) m' 0,y,z  
(1 0,0,0)'  
(15) m' x+1/2,x,z  
(1 1/2,1/2,0)'  
(16) g' (1/2,1/2,0) x,x,z  
(1 1/2,1/2,0)'

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

16 k 11'

(1) x,y,z [0,0,0]  
(2) x,y,z [0,0,0]  
(3) y+1/2,x+1/2,z [0,0,0]  
(4) y+1/2,x+1/2,z [0,0,0]

(5) x+1/2,y+1/2,z [0,0,0]  
(6) x+1/2,y+1/2,z [0,0,0]  
(7) y,x,z [0,0,0]  
(8) y,x,z [0,0,0]

(9) x+1/2,y+1/2,z [0,0,0]  
(10) x+1/2,y+1/2,z [0,0,0]  
(11) y,x,z [0,0,0]  
(12) y,x,z [0,0,0]

(13) x,y,z [0,0,0]  
(14) x,y,z [0,0,0]  
(15) y+1/2,x+1/2,z [0,0,0]  
(16) y+1/2,x+1/2,z [0,0,0]

8 j m1' x,x+1/2,z [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)

8 i m1' 0,y,z [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)

8 h 21' x,x,1/2 [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)

8 g 21' x,x,0 [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)

4 f 2mm.1' 0,0,z [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)

4 e 2/m1' 1/4,1/4,1/2 [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)

4 d 2/m1' 1/4,1/4,0 [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)

2 c 4mm1' 0,1/2,z [0,0,0]  
(0,0,0)  
(0,0,0)  
(0,0,0)  
(0,0,0)
Continued

2 b $\bar{4}m21'$ 0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]
2 a $\bar{4}m21'$ 0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'
$a^* = (a - b)/2$  $b^* = (a + b)/2$
Origin at 0,0,z

Along [1,0,0] p2mg1'
$a^* = b$  $b^* = c$
Origin at x,1/4,0

Along [1,1,0] p2mm1'
$a^* = (-a + b)/2$  $b^* = c$
Origin at x,x,0
Origin at center $\overline{4}'m2'$ at $\overline{4}'/nm2'/g$, at -1/4,1/4,0 from center (2'/m)

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

Symmetry Operations

(1) 1
(1 | 0,0,0)

(5) 2' (0,1/2,0) 1/4,y,0
(2z | 1/2,1/2,0)'

(9) $\overline{1}'$ 1/4,1/4,0
(1 | 1/2,1/2,0)'

(13) m x,0,z
(m | 0,0,0)

(2) 2 0,0,z
(2z | 0,0,0)

(6) 2' (1/2,1/2,0) x,1/4,0
(2z | 1/2,1/2,0)'

(10) n' (1/2,1/2,0) x,y,0
(m | 1/2,1/2,0)'

(14) m 0,y,z
(m | 0,0,0)

(3) $4'$ 0,1/2,z
(4z | 1/2,1/2,0)

(7) 2' x,x,0
(2x | 0,0,0)'

(11) $\overline{4}'$ * 0,0,z; 0,0,0
(4z | 0,0,0)'

(15) m x+1/2,x,z
(m | 1/2,1/2,0)

(4) $4'$ 1/2,0,z
(4z | 1/2,1/2,0)

(8) 2' x,x,0
(2x | 0,0,0)'

(12) $\overline{4}'$ * 0,0,z; 0,0,0
(4z | 0,0,0)'

(16) g (1/2,1/2,0) x,x,z
(m | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>k</td>
</tr>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>u,v,w</td>
</tr>
<tr>
<td>(2) x,y,z</td>
<td>u,v,w</td>
</tr>
<tr>
<td>(3) y+1/2,x+1/2,z</td>
<td>v,u,w</td>
</tr>
<tr>
<td>(4) y+1/2,x+1/2,z</td>
<td>v,u,w</td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z</td>
<td>u,v,w</td>
</tr>
<tr>
<td>(6) x+1/2,y+1/2,z</td>
<td>u,v,w</td>
</tr>
<tr>
<td>(7) y,x,z</td>
<td>v,u,w</td>
</tr>
<tr>
<td>(8) y,x,z</td>
<td>v,u,w</td>
</tr>
<tr>
<td>(9) x+1/2,y+1/2,z</td>
<td>u,v,w</td>
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<tr>
<td>(10) y+1/2,x+1/2,z</td>
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<td>(13) x,y,z</td>
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<td>(14) x,y,z</td>
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<td>(15) y+1/2,x+1/2,z</td>
<td>v,u,w</td>
</tr>
<tr>
<td>(16) y+1/2,x+1/2,z</td>
<td>v,u,w</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p 4'mm'  a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0]  p 2mm  a* = b  b* = c
Origin at x,1/4,0

Along [1,1,0]  p 2mm'  a* = (a - b)/2  b* = c
Origin at x,x,0
Origin at center $\overline{4}m2$ at $\overline{4}'/nm2/g$, at $-1/4,1/4,0$ from center ($2/m$).

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

Symmetry Operations

(1) $1$

(2) $2$ $0,0,z$

(3) $4'$ $0,1/2,z$

(4) $4' \cdot 1/2,0,z$

(5) $2'$ $(0,1/2,0)$ $1/4,y,0$

(6) $2' (1/2,0,0)$ $x,1/4,0$

(7) $2 \cdot x,x,0$

(8) $2 \cdot x,x,0$

(9) $\overline{4}$ $1/4,1/4,0$

(10) $n (1/2,1/2,0)$ $x,y,0$

(11) $\overline{4} \cdot 0,0,z; 0,0,0$

(12) $\overline{4} \cdot 0,0,z; 0,0,0$

(13) $\overline{4}$ $x,0,z$

(14) $m' 0,y,z$

(15) $m \cdot x+1/2,\overline{x},z$

(16) $g (1/2,1/2,0)$ $x,x,z$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

16 k 1

(1) x,y,z [u,v,w]  (2) x',y',z [u',v',w']  (3) y+1/2,x+1/2,z [v,u,w]  (4) y+1/2,x+1/2,z [v,u,w]  
(5) x+1/2,y+1/2,z [u,v,w]  (6) x+1/2,y+1/2,z [u,v,w]  (7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]  
(9) x+1/2,y+1/2,z [u,v,w]  (10) x+1/2,y+1/2,z [u,v,w]  (11) y,x,z [v,u,w]  (12) y,x,z [v,u,w]  
(13) x,y,z [u,v,w]  (14) x,y,z [u,v,w]  (15) y+1/2,x+1/2,z [v,u,w]  (16) y+1/2,x+1/2,z [v,u,w]  

8 j .m  x+1/2,z [u,u,0]  x,x+1/2,z [u,u,0]  x,x+1/2,z [u,u,0]  x,x+1/2,z [u,u,0]  
8 i .m': 0,y,z [0,v,w]  0,y,z [0,v,w]  y+1/2,1/2,z [v,0,w]  y+1/2,1/2,z [v,0,w]  
8 h .2  x,x,1/2 [u,u,0]  x,x,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  x+1/2,x+1/2,1/2 [u,u,0]  

8 g .2  x,x,0 [u,u,0]  x,x,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  
4 f 2m'm'. 0,0,z [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]  0,0,z [0,0,w]  
4 e .2/m  1/4,1/4,1/2 [u,u,0]  3/4,3/4,1/2 [u,u,0]  1/4,3/4,1/2 [u,u,0]  3/4,1/4,1/2 [u,u,0]  
4 d .2/m  1/4,1/4,0 [u,u,0]  3/4,3/4,0 [u,u,0]  1/4,3/4,0 [u,u,0]  3/4,1/4,0 [u,u,0]  
2 c 4'm'm'  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  
2 b 4'm'2  0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  0,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  
2 a 4'm'2  0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]  0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1]  p'c, 4'm'm'  \( a^* = (a - b) / 2 \), \( b^* = (a + b) / 2 \)  
Origin at 0,0,0  
Along [1,0,0]  p2m'g'  \( a^* = b \), \( b^* = c \)  
Origin at x,1/4,0  
Along [1,1,0]  p2mm1'  \( a^* = -(a + b) / 2 \), \( b^* = c \)  
Origin at x,x,0  

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Origin at center $\overline{4}m2'$ at $\overline{4}'/nm2'/g'$, at $-1/4,1/4,0$ from center ($2'/m'$)

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

Symmetry Operations

(1) $1$

$\bar{1} \ 0,0,0$

(2) $2 \ 0,0,z$

$2_z \ 0,0,0$

(3) $4' \ 0,1/2,z$

$4_z \ 1/2,1/2,0'$

(4) $4' \ 1/2,0,z$

$4_z \ 1/2,1/2,0'$

(5) $2 \ (0,1/2,0) \ 1/4,y,0$

$2_z \ 1/2,1/2,0$

(6) $2 \ (1/2,0,0) \ x,1/4,0$

$2_z \ 1/2,1/2,0$

(7) $2' \ x,x,0$

$2_{xy} \ 0,0,0'$

(8) $2' \ x,x,0$

$2_{xy} \ 0,0,0'$

(9) $\bar{1} \ 1/4,1/4,0$

$\bar{1} \ 1/2,1/2,0$

(10) $n \ (1/2,1/2,0) \ x,y,0$

$m_z \ 1/2,1/2,0$

(11) $\bar{4}' \ 0,0,z; \ 0,0,0$

$\bar{4}_z \ 0,0,0'$

(12) $\bar{4}' \ 0,0,z; \ 0,0,0$

$\bar{4}_z \ 0,0,0'$

(13) $m \ x,0,z$

$m \ 0,0,0$

(14) $m \ 0,y,z$

$m \ 0,0,0$

(15) $m' \ x+1/2,x,z$

$m_{xy} \ 1/2,1/2,0'$

(16) $g' \ (1/2,1/2,0) \ x,x,z$

$m_{xy} \ 1/2,1/2,0'$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>16</td>
<td>k</td>
</tr>
<tr>
<td>(2) x,y,z [u,v,w]</td>
<td>8</td>
<td>j</td>
</tr>
<tr>
<td>(3) y+1/2,x+1/2,z [v,u,w]</td>
<td>8</td>
<td>i</td>
</tr>
<tr>
<td>(4) y+1/2,x+1/2,z [v,u,w]</td>
<td>8</td>
<td>h</td>
</tr>
<tr>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>4</td>
<td>f</td>
</tr>
<tr>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
<td>4</td>
<td>e</td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>4</td>
<td>d</td>
</tr>
<tr>
<td>(8) y,x,z [v,u,w]</td>
<td>2</td>
<td>c</td>
</tr>
<tr>
<td>(9) x+1/2,y+1/2,z [u,v,w]</td>
<td>2</td>
<td>b</td>
</tr>
<tr>
<td>(10) y+1/2,x+1/2,z [v,u,w]</td>
<td>2</td>
<td>a</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'mmm
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] p2mg1'
\[ a^* = b \quad b^* = c \]
Origin at x,1/4,0

Along [1,1,0] p2'mmm'
\[ a^* = -c \quad b^* = (-a + b)/2 \]
Origin at x,x,0
P4'/n'm'm  
129.6.1080

4'/m'm'm  
P4'/n'2,./m'2'/m
Tetragonal

Origin at center 4m'2' at 4/n'm'2'/g, at -1/4,1/4,0 from center (2'/m)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

(1) 1
(1) 0,0,0
(1|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(3) 4+ 0,1/2,z
(4z|1/2,1/2,0)

(4) 4+ 1/2,0,z
(4z|1/2,1/2,0)

(5) 2 (0,1/2,0) 1/4,y,0
(2,1/2,1/2,0)

(6) 2 (1/2,0,0) x,1/4,0
(2x,1/2,1/2,0)

(7) 2' x,x,0
(2xx|0,0,0)

(8) 2' x,x,0
(2xx|0,0,0)

(9) 1/4,1/4,0
(1|1/2,1/2,0)

(10) n' (1/2,1/2,0) x,y,0
(m,1/2,1/2,0)

(11) 4' 0,0,z; 0,0,0
(4z|0,0,0)

(12) 4' 0,0,z; 0,0,0
(4z|0,0,0)

(13) m' x,0,z
(m,0,0,0)

(14) m' 0,y,z
(m,0,0,0)

(15) m x+1/2,x,z
(m,1/2,1/2,0)

(16) g (1/2,1/2,0) x,x,z
(mx,1/2,1/2,0)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>k</td>
<td>1</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Coordinates

<table>
<thead>
<tr>
<th>Position</th>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z [v,u,w]</td>
<td>(4) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x+1/2,y+1/2,z [u,v,w]</td>
<td>(10) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(11) y,x,z [v,u,w]</td>
<td>(12) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(13) x,y,z [u,v,w]</td>
<td>(14) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(15) y+1/2,x+1/2,z [v,u,w]</td>
<td>(16) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4'm'm

\[ a^* = (\mathbf{a} - \mathbf{b})/2 \]

Origin at 0,0,z

Along [1,0,0] p2m'g'

\[ a^* = \mathbf{a} \quad b^* = \mathbf{b} \]

Origin at x,1/4,0

Along [1,1,0] p2mm'1

\[ a^* = (-\mathbf{a} + \mathbf{b})/2 \quad b^* = \mathbf{c} \]

Origin at x,x,0
Origin at center $\overline{4}m'2'$ at $\overline{4}/nm'2'/g'$, at -1/4,1/4,0 from center ($2'/m'$)

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ 1/2 - x

Symmetry Operations

(1) 1
(1 | 0,0,0)

(5) 2' (0,1/2,0) 1/4,y,0
(2_z | 1/2,1/2,0)

(9) T 1/4,1/4,0
(1 | 1/2,1/2,0)

(13) m' x,0,z
(m_y | 0,0,0)

(2) 2 0,0,z
(2_z | 0,0,0)

(6) 2' (1/2,0,0) x,1/4,0
(2_z | 1/2,1/2,0)

(10) n (1/2,1/2,0) x,y,0
(m_z | 1/2,1/2,0)

(14) m' 0,y,z
(m_z | 0,0,0)

(3) 4' 0,1/2,z
(4_z | 1/2,1/2,0)

(7) 2' x,x,0
(2_y | 0,0,0)

(11) 4' 0,0,z; 0,0,0
(4_z | 0,0,0)

(15) m' x+1/2,x,z
(m_y | 1/2,1/2,0)

(4) 4' 1/2,0,z
(4_z | 1/2,1/2,0)

(8) 2' x,x,0
(2_y | 0,0,0)

(12) 4'; 0,0,z; 0,0,0
(4_z | 0,0,0)

(16) g' (1/2,1/2,0) x,x,z
(m_y | 1/2,1/2,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

\begin{align*}
16 & \begin{array}{llll}
1 & (1) & x,y,z & [u,v,w] \\
(2) & x',y',z' & [u',v',w] \\
(3) & y+1/2,x+1/2,z & [v,u,w] \\
(4) & y+1/2,x+1/2,z & [v,u,w] \\
(5) & x+1/2,y+1/2,z & [u,v,w] \\
(6) & x+1/2,y+1/2,z & [u,v,w] \\
(7) & y,x,z & [v,u,w] \\
(8) & y,x,z & [v,u,w] \\
(9) & x+1/2,y+1/2,z & [u,v,w] \\
(10) & x+1/2,y+1/2,z & [u,v,w] \\
(11) & y,x,z & [v,u,w] \\
(12) & y,x,z & [v,u,w] \\
(13) & x,y,z & [u,v,w] \\
(14) & x,y,z & [u,v,w] \\
(15) & y+1/2,x+1/2,z & [v,u,w] \\
(16) & y+1/2,x+1/2,z & [v,u,w] \\
8 & j & m' & x,x+1/2,z & [u,u,w] \\
& & & x,x+1/2,z & [u,u,w] \\
& & & x,x+1/2,z & [u,u,w] \\
8 & i & m'. & 0,y,z & [0,v,w] \\
& & & 0,y,z & [0,v,w] \\
& & & 0,y,z & [0,v,w] \\
8 & h & 2' & x,x+1/2 & [u,u,w] \\
& & & x,x+1/2 & [u,u,w] \\
& & & x,x+1/2 & [u,u,w] \\
8 & g & 2' & x,x,0 & [u,u,w] \\
& & & x,x,0 & [u,u,w] \\
& & & x,x,0 & [u,u,w] \\
4 & f & 2m'. & 0,0,z & [0,0,w] \\
& & & 1/2,1/2,z & [0,0,w] \\
& & & 1/2,1/2,z & [0,0,w] \\
4 & e & 2'/m' & 1/4,1/4,1/2 & [u,u,w] \\
& & & 3/4,3/4,1/2 & [u,u,w] \\
& & & 3/4,3/4,1/2 & [u,u,w] \\
4 & d & 2'/m' & 1/4,1/4,0 & [u,u,w] \\
& & & 3/4,3/4,0 & [u,u,w] \\
& & & 3/4,3/4,0 & [u,u,w] \\
2 & c & 4m'. & 0,1/2,z & [0,0,w] \\
& & & 1/2,0,z & [0,0,w] \\
2 & b & 4m'2' & 0,0,1/2 & [0,0,w] \\
& & & 1/2,1/2,1/2 & [0,0,w] \\
2 & a & 4m'2' & 0,0,0 & [0,0,w] \\
& & & 1/2,1/2,0 & [0,0,w]
\end{array}
\end{align*}

Symmetry of Special Projections

Along [0,0,1]  \( p_{0.2} \) 4m'm'
Along [1,0,0]  \( p_{2} \) 4m'g
Along [1,1,0]  \( p_{2mm} \) 4m'

\[ a^* = (a-b)/2 \quad b^* = (a+b)/2 \]

Origin at 1/2,0,z

\[ a^* = b \quad b^* = c \]

Origin at x,1/4,0

\[ a^* = c \quad b^* = -(a+b)/2 \]

Origin at x,x,0
Origin at center $\overline{4}m\bar{2}$ at $\overline{4}/n'm2/g'$, at $-1/4,1/4,0$ from center ($2/m'$)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

Symmetry Operations

1. 1
2. $2,0,0,z$ $0 \leq z \leq 1/2$
3. $4^+,0,1/2,z$ $0 \leq z \leq 1/2$
4. $4^+,1/2,0,z$ $0 \leq z \leq 1/2$
5. $2'(0,1/2,0)$ $1/4,y,0$ $0 \leq y \leq 1/2$
6. $2'(1/2,0,0)$ $2',1/2,0$ $0 \leq y \leq 1/2$
7. $2,x,x,0$ $0 \leq x \leq 1/2$
8. $2,x,x,0$ $0 \leq x \leq 1/2$
9. $\overline{1}^+,1/4,1/4,0$ $x,1/4,0$ $0 \leq z \leq 1/2$
10. $\overline{1}^+,1/2,1/2,0$ $x,1/4,0$ $0 \leq z \leq 1/2$
11. $\overline{4}^-,0,0,z$ $0 \leq z \leq 1/2$
12. $\overline{4}^-,0,0,z$ $0 \leq z \leq 1/2$
13. $m,x,0,z$ $0 \leq z \leq 1/2$
14. $m,0,y,z$ $0 \leq y \leq 1/2$
15. $m',x+1/2,x,z$ $0 \leq z \leq 1/2$
16. $g'(1/2,1/2,0)$ $x,x,z$ $0 \leq z \leq 1/2$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Number</th>
<th>k</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td></td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>(3) y+1/2, x+1/2, z [v, u, w]</td>
<td>(4) y+1/2, x+1/2, z [v, u, w]</td>
</tr>
<tr>
<td>(5) x+1/2, y+1/2, z [u, v, w]</td>
<td>(6) x+1/2, y+1/2, z [u, v, w]</td>
</tr>
<tr>
<td>(7) y, x, z [v, u, w]</td>
<td>(8) y, x, z [v, u, w]</td>
</tr>
<tr>
<td>(9) x, y, z [u, v, w]</td>
<td>(10) x, y, z [u, v, w]</td>
</tr>
</tbody>
</table>

Along [0,0,1] p 4'm'm
a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2mg1'
a* = b  b* = c
Origin at x,1/4,0

Along [1,1,0] p2'mm'
a* = -c  b* = (-a + b)/2
Origin at x,x,0

Symmetry of Special Projections
Along [0,0,1] p 4'm'm
a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2mg1'
a* = b  b* = c
Origin at x,1/4,0

Along [1,1,0] p2'mm'
a* = -c  b* = (-a + b)/2
Origin at x,x,0
Origin at center \(\overline{4}m'2\) at \(\overline{4}'\overline{n}'m'2\overline{g}'\), at -1/4,1/4,0 from center (2/m')

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x
\]

Symmetry Operations

\begin{align*}
(1) & \quad 1
(1\parallel 0,0,0) \\
(5) & \quad 2 \quad (0,1/2,0) \quad 1/4,y,0 \\
& \quad (2\parallel 1/2,1/2,0) \\
(9) & \quad \overline{1} \quad 1/4,1/4,0 \\
& \quad (1\parallel 1/2,1/2,0)' \\
(13) & \quad m' \quad x,0,z \\
& \quad (m\parallel 0,0,0)' \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2z\parallel 0,0,0) \\
(6) & \quad 2 \quad (1/2,0,0) \quad x,1/4,0 \\
& \quad (2x\parallel 1/2,1/2,0) \\
(10) & \quad n' \quad (1/2,1/2,0) \quad x,y,0 \\
& \quad (m\parallel 1/2,1/2,0)' \\
(14) & \quad m' \quad 0,y,z \\
& \quad (m\parallel 0,0,0)' \\
(3) & \quad 4' \quad 0,1/2,z \\
& \quad (4z\parallel 1/2,1/2,0) \\
(7) & \quad 2 \quad x,x,0 \\
& \quad (2x\parallel 0,0,0) \\
(11) & \quad 4' \quad 0,0,z; 0,0,0 \\
& \quad (4z\parallel 0,0,0)' \\
(15) & \quad m' \quad x+1/2,x,z \\
& \quad (m\parallel 1/2,1/2,0)' \\
(4) & \quad 4' \quad 1/2,0,z \\
& \quad (4z\parallel 1/2,1/2,0) \\
(8) & \quad 2 \quad x,\overline{x},0 \\
& \quad (2x\parallel 0,0,0) \\
(12) & \quad 4' \quad 0,0,z; 0,0,0 \\
& \quad (4z\parallel 0,0,0)' \\
(16) & \quad g' \quad (1/2,1/2,0) \quad x,x,z \\
& \quad (m\parallel 1/2,1/2,0)' \\
\end{align*}
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>k</td>
<td>1</td>
</tr>
</tbody>
</table>

Positions are given as multiples of the translation vectors, with Wyckoff letters indicating the symmetry operations. The coordinates include translations and rotations.

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at 0,0,z</th>
<th>Along [0,0,1]</th>
<th>p4m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>a* = b</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Origin at x,1/4,0</th>
<th>Along [1,0,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b</td>
<td>a* = b</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Origin at x,x,0</th>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/2</td>
<td>a* = b</td>
<td>b* = c</td>
</tr>
</tbody>
</table>
Origin at center \( \overline{4} m 2 \) at \( \overline{4}/n m 2/g \), at \(-1/4,1/4,0\) from center (2/\(m\))

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x \]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 \\
 & \quad (1 | 0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
 & \quad (2_z | 0,0,0) \\
(3) & \quad 4^+ \quad 0,1/2,z \\
 & \quad (4_z | 1/2,1/2,0) \\
(4) & \quad 4^+ \quad 1/2,0,z \\
 & \quad (4_z^{-1} | 1/2,1/2,0) \\
(5) & \quad 2 \quad (0,1/2,0) \quad 1/4,y,0 \\
 & \quad (2_z | 1/2,1/2,0) \\
(6) & \quad 2 \quad (1/2,0,0) \quad x,1/4,0 \\
 & \quad (2_x | 1/2,1/2,0) \\
(7) & \quad 2 \quad x,x,0 \\
 & \quad (2_{xy} | 0,0,0) \\
(8) & \quad 2 \quad x,x,0 \\
 & \quad (2_{xy} | 0,0,0) \\
(9) & \quad \overline{4} \quad 1/4,1/4,0 \\
 & \quad (\overline{4} | 1/2,1/2,0) \\
(10) & \quad n \quad (1/2,1/2,0) \quad x,y,0 \\
 & \quad (m_{z-1/2} | 1/2,1/2,0) \\
(11) & \quad \overline{4} \quad 0,0,z \quad 0,0,0 \\
 & \quad (\overline{4}_z | 0,0,0) \\
(12) & \quad \overline{4} \quad 0,0,z \quad 0,0,0 \\
 & \quad (\overline{4}_z^{-1} | 0,0,0) \\
(13) & \quad m \quad x,0,z \\
 & \quad (m_{0,0,0}) \\
(14) & \quad m \quad 0,y,z \\
 & \quad (m_{0,0,0}) \\
(15) & \quad m \quad x+1/2,\overline{x},z \\
 & \quad (m_{x+1/2,1/2,0}) \\
(16) & \quad g \quad (1/2,1/2,1) \quad x,x,z \\
 & \quad (m_{x+1/2,1/2,0})
\end{align*}
\]

For (0,0,1) + set

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
 & \quad (1 | 0,0,1)' \\
(2) & \quad 2' \quad (0,0,1) \quad 0,0,z \\
 & \quad (2_z | 0,0,1)' \\
(3) & \quad 4^+ \quad (0,0,1) \quad 0,1/2,z \\
 & \quad (4_z | 1/2,1/2,1)' \\
(4) & \quad 4^+ \quad (0,0,1) \quad 1/2,0,z \\
 & \quad (4_z^{-1} | 1/2,1/2,1)' \\
(5) & \quad 2' \quad (0,1/2,0) \quad 1/4,y,1/2 \\
 & \quad (2_z | 1/2,1/2,1)'
\end{align*}
\]

Generators selected

\( (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
(0,0,0) + (0,0,1)' +
\end{align*}
\]

\[
\begin{align*}
(1) & \quad x,y,z \ [u,v,w] \\
(2) & \quad \overline{x},\overline{y},\overline{z} \ [\overline{u},\overline{v},\overline{w}] \\
(3) & \quad y+1/2,x+1/2,z \ [\overline{v},u,w] \\
(4) & \quad y+1/2,\overline{x}+1/2,z \ [\overline{v},u,w] \\
(5) & \quad x+1/2,y+1/2,\overline{z} \ [u,v,w] \\
(6) & \quad x+1/2,\overline{y}+1/2,\overline{z} \ [u,v,w] \\
(7) & \quad y,x,z \ [v,u,w] \\
(8) & \quad \overline{y},\overline{x},z \ [\overline{v},u,w] \\
(9) & \quad \overline{x}+1/2,y+1/2,\overline{z} \ [u,v,w] \\
(10) & \quad x+1/2,y+1/2,\overline{z} \ [\overline{u},\overline{v},w] \\
(11) & \quad y,x,z \ [v,u,w] \\
(12) & \quad \overline{y},\overline{x},z \ [\overline{v},u,w] \\
(13) & \quad x,\overline{y},z \ [u,v,w] \\
(14) & \quad \overline{x},\overline{y},\overline{z} \ [\overline{u},\overline{v},\overline{w}] \\
(15) & \quad \overline{y}+1/2,\overline{x}+1/2,z \ [v,u,w] \\
(16) & \quad y+1/2,\overline{x}+1/2,z \ [\overline{v},u,w]
\end{align*}
\]
Continued 129.10.1084

16  i  .m.  0,y,z [u,0,0]  0,y ,z [u,0,0]  y+1/2,1/2,z [0,u,0]  y+1/2,1/2,z [0,u,0]  
    1/2,y+1/2,z [u,0,0]  1/2,y+1/2,z [u,0,0]  y,0,z [0,u,0]  y,0,z [0,u,0]  
16  h  ..2'  x,x,1/2 [u,u,w]  x,x,1/2 [u,u,w]  x+1/2,x+1/2,1/2 [u,u,w]  x+1/2,x+1/2,1/2 [u,u,w]  
    x+1/2,x+1/2,1/2 [u,u,w] x,x,1/2 [u,u,w]  x,x,1/2 [u,u,w]  
16  g  ..2  x,x,0 [u,u,0]  x,x,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  
    x+1/2,x+1/2,0 [u,u,0] x,x,0 [u,u,0]  x,x,0 [u,u,0]  
 8   f  2mm.  0,0,z [0,0,0]  1/2,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]  0,0,z [0,0,0]  
 8   e  ..2'/m  1/4,1/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]  
 8   d  ..2/m  1/4,1/4,0 [u,u,0]  3/4,3/4,0 [u,u,0]  1/4,3/4,0 [u,u,0]  3/4,1/4,0 [u,u,0]  
 4   c  4mm  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  
 4   b  4'm2'  0,0,1/2 [0,0,0]  1/2,1,2,1/2 [0,0,0]  
 4   a  4m2  0,0,0 [0,0,0]  1/2,1,2,0 [0,0,0]  

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p 4mm 1'</th>
<th>Along [1,0,0]</th>
<th>p2mg 1'</th>
<th>Along [1,1,0]</th>
<th>p2mm 1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>a* = b</td>
<td>b* = c</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  Origin at x,1/4,0  Origin at x,x,0
Origin at center $\overline{4}m^2$ at $\overline{4}'/nm^2$g, at -1/4, 1/4, 0 from center (2/m)

Asymmetric unit
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x$

Symmetry Operations

For (0,0,0) + set

1. $1$
2. $2 \times 0,0,z$
3. $4+ \times 0,1/2,z$
4. $4- \times 1/2,0,z$
5. $2' \times (0,1/2,0), \quad 1/4, y, 0$
6. $2' \times (1/2,0,0), \quad x, 1/4, 0$
7. $2' \times x, x, 0$
8. $2' \times x, x, 0$
9. $1 \times y, y, 0$
10. $1 \times y, y, 0$
11. $4+ \times 0,0, z; 0,0, 0$
12. $4+ \times 0,0, z; 0,0, 0$
13. $m' \times x, 0, z$
14. $m' \times 0, y, z$
15. $m' \times x+1/2, x, z$
16. $g \times 1/2, 1/2, 0$

For (0,0,1) + set

1. $t' \times (0,0,1)$
2. $2' \times (0,0,1), \quad 0,0,z$
3. $4+ \times (0,0,1), \quad 0,1/2,z$
4. $4+ \times 0,0, z; 0,0, 1/2$
5. $2 \times (0,1/2,0), \quad 1/4, y, 1/2$
6. $2 \times (1/2,0,0), \quad x, 1/4, 1/2$
7. $2' \times x, x, 1/2$
8. $2' \times x, x, 1/2$
9. $1 \times y, y, 1/2$
10. $1 \times y, y, 1/2$
11. $4+ \times 0,0, z; 0,0, 0$
12. $4+ \times 0,0, z; 0,0, 1/2$
13. $c \times (0,0,1), \quad x, 0, z$
14. $c \times (0,0,1), \quad 0, y, z$
15. $c' \times (0,0,1), \quad x+1/2, x, z$
16. $n' \times (1/2,1/2,1), \quad x, x, z$

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

32 $k \times 1$

(1) $x, y, z$ [u,v,w]
(2) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]
(3) $y+1/2, x+1/2, z$ [v,u,w]
(4) $y+1/2, x+1/2, z$ [v,u,w]
(5) $x+1/2, y+1/2, z$ [u,v,w]
(6) $x+1/2, y+1/2, z$ [u,v,w]
(7) $y, x, z$ [v,u,w]
(8) $y, x, z$ [v,u,w]
(9) $x+1/2, y+1/2, z$ [u,v,w]
(10) $x+1/2, y+1/2, z$ [u,v,w]
(11) $y, x, z$ [v,u,w]
(12) $y, x, z$ [v,u,w]
(13) $x, y, z$ [u,v,w]
(14) $\bar{x}, \bar{y}, \bar{z}$ [u,v,w]
(15) $\bar{y}+1/2, x+1/2, z$ [v,u,w]
(16) $y+1/2, x+1/2, z$ [v,u,w]

16 $j \times . m$

(1) $x, x+1/2, z$ [u,u,0]
(2) $\bar{x}, \bar{x}+1/2, z$ [u,u,0]
(3) $x, x+1/2, z$ [u,u,0]
(4) $\bar{x}, \bar{x}+1/2, z$ [u,u,0]
(5) $x, x+1/2, z$ [u,u,0]
(6) $\bar{x}, \bar{x}+1/2, z$ [u,u,0]
(7) $x, x+1/2, z$ [u,u,0]
(8) $\bar{x}, \bar{x}+1/2, z$ [u,u,0]
16  i  .m'.  0,y,z [0,v,w]  0,y,z [0,v,w]  y+1/2,1/2,z [v,0,w]  y+1/2,1/2,z [v,0,w]  
1/2,y+1/2,z [0,v,w]  1/2,y+1/2,z [0,v,w]  y,0,z [v,0,w]  y,0,z [v,0,w]  
16  h  .2'  x,x,1/2 [u,u,w]  x,x,1/2 [u,u,w]  x+1/2,x+1/2,1/2 [u,u,w]  x+1/2,x+1/2,1/2 [u,u,w]  
  x+1/2,x+1/2,1/2 [u,u,w]  x,x,1/2 [u,u,w]  x,x,1/2 [u,u,w]  x+1/2,x+1/2,1/2 [u,u,w]  
16  g  .2  x,x,0 [u,u,0]  x,x,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  
  x+1/2,x+1/2,0 [u,u,0]  x+1/2,x+1/2,0 [u,u,0]  x,x,0 [u,u,0]  x,x,0 [u,u,0]  
8   f  2m'm'.  0,0,z [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]  0,0,z [0,0,w]  
8   e  .2'/m  1/4,1/4,1/2 [0,0,0]  3/4,3/4,1/2 [0,0,0]  1/4,3/4,1/2 [0,0,0]  3/4,1/4,1/2 [0,0,0]  
8   d  .2/m  1/4,1/4,0 [u,u,0]  3/4,3/4,0 [u,u,0]  1/4,3/4,0 [u,u,0]  3/4,1/4,0 [u,u,0]  
4   c  4'm'm  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  
4   b  4'm'2'  0,0,1/2 [0,0,w]  1/2,1/2,1/2 [0,0,w]  
4   a  4'm'2  0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1]  p 4mm1'  Along [1,0,0]  p 2m'g'  Along [1,1,0]  p 2mm1'
\( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  \( a^* = b \)  \( b^* = c \)  \( a^* = (-a + b)/2 \)  \( b^* = c \)
Origin at 0,0,z  Origin at x,1/4,1/2  Origin at x,x,0
P_2c 4'/nmm'

4/mmm1'

Tetragonal

129.12.1086

P_2c 4'/n2_1/m2_1/m'
Origin at center \( \overline{4}m2' \) at \( \overline{4}'nm2'/g' \), at -1/4,1/4,0 from center (2'/m')

Asymmetric unit  
\( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq 1/2 - x \)

Symmetry Operations

For \((0,0,0)+\) set

\[
\begin{align*}
(1) \quad & x, y, z \quad [u, v, w] \\
(2) \quad & x+y+1/2, x+1/2, z + v+1/2, [u, v, w] \\
(3) \quad & y+1/2, x+1/2, z + [v, u, w] \\
(4) \quad & y+1/2, x+1/2, z + [v, u, w] \\
(5) \quad & x+1/2, y+1/2, z + [u, v, w] \\
(6) \quad & x+y+1/2, y+1/2, z + [u, v, w] \\
(7) \quad & y, x, z + v, u, w \\
(8) \quad & y, x, z + v, u, w \\
(9) \quad & x+y+1/2, x+1/2, z + [u, v, w] \\
(10) \quad & x+y+1/2, x+1/2, z + [u, v, w] \\
(11) \quad & y, x, z + v, u, w \\
(12) \quad & y, x, z + v, u, w \\
(13) \quad & x, y, z + [u, v, w] \\
(14) \quad & x, y, z + [u, v, w] \\
(15) \quad & y+1/2, x+1/2, z + [v, u, w] \\
(16) \quad & y+1/2, x+1/2, z + [v, u, w] \\
\end{align*}
\]

Generators selected \((1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (3); (5); (9).\)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
32 & \quad \begin{array}{ll}
32 & \quad k & \quad 1 \\
(1) & \quad x, y, z + [u, v, w] \\
(5) & \quad x+y+1/2, y+1/2, z + [u, v, w] \\
(9) & \quad x+y+1/2, x+1/2, z + [u, v, w] \\
(13) & \quad x, y, z + [u, v, w] \\
\end{array} \\
16 & \quad \begin{array}{ll}
16 & \quad j & \quad m' \\
\end{array} \\
\end{align*}
\]
16 i .m. 0,y,z [u,0,0] 0,y,z [0-u,0] y+1/2,1/2,z [0,u,0] y+1/2,1/2,z [0,u,0] 1/2,y+1/2,z [u,0,0] 1/2,y+1/2,z [u,0,0] y,0,z [0,u,0] y,0,z [0,u,0] 16 h .2 x,x,1/2 [u,u,0] x+1/2,y+1/2,z [u,0,0] x+1/2,y+1/2,z [u,0,0] y,0,z [0,u,0] y,0,z [0,u,0] 1/2,y+1/2,z [u,0,0] 1/2,y+1/2,z [u,0,0] 16 g .2' x,x,0 [u,u,w] x+1/2,x+1/2,0 [u,u,w] x+1/2,x+1/2,0 [u,u,w] x+1/2,x+1/2,0 [u,u,w] x+1/2,x+1/2,0 [u,u,w] x,x,0 [u,u,w] 1/2,y+1/2,z [0,u,0] 1/2,y+1/2,z [0,u,0] 8 f 2mm. 0,0,z [0,0,0] 1/2,1/2,z [0,0,0] 1/2,1/2,z [0,0,0] 0,0,z [0,0,0] 8 e .2/m 1/2,1/2,0 [u,u,0] 3/4,1/2,1/2 [u,u,0] 3/4,1/2,1/2 [u,u,0] 1/2,1/2,0 [u,u,0] 1/2,1/2,0 [u,u,0] 8 d .2'/m' 1/2,1/2,0 [u,u,0] 3/4,3/4,0 [u,u,0] 3/4,3/4,0 [u,u,0] 1/2,1/2,0 [u,u,0] 1/2,1/2,0 [u,u,0] 4 c 4'mm' 0,1/2,z [0,0,0] 1/2,0,z [0,0,0] 1/2,0,z [0,0,0] 4 b 4'm2 0,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0] 4 a 4'm2' 0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] Symmetry of Special Projections

Along [0,0,1] p4mm1'
\[ a^* = \frac{a - b}{2} \quad b^* = \frac{a + b}{2} \]
Origin at 0,0,z

Along [1,0,0] p2mg1'
\[ a^* = b \quad b^* = c \]
Origin at x,1/4,0

Along [1,1,0] p2na 2m'm'
\[ a^* = -c \quad b^* = \frac{-a + b}{2} \]
Origin at x,x,1/2

129.12.1086 - 3 - 2234
Origin at center $\overline{4}m2'$ at $\overline{4}/nm2'/g'$, at -1/4,1/4,0 from center ($2'/m'$).

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2; y \leq 1/2 - x$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1
(2) $2' (0,0,1)$
(5) $2' (0,1/2,0)$
(9) $1'$
(12) $4'$
(13) $m'$
(16) $g'$

(1)' + set

(1) $t'(0,0,1)$
(2) $2' (0,0,1)$
(5) $2 (0,1/2,0)$
(9) $1'$
(13) $c (0,0,1)$
(16) $n (1/2,1/2,1)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t'(0,0,1)$; (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

$$(0,0,0) + (0,0,1)' +$$

32 $k$ 1

(1) $x,y,z [u,v,w]$ (2) $x,y,z [u,v,w]$ (3) $y+1/2,x+1/2,z [v,u,w]$ (4) $y+1/2,x+1/2,z [v,u,w]$

(5) $x+1/2,y+1/2,z [u,v,w]$ (6) $x+1/2,y+1/2,z [u,v,w]$ (7) $y,x,z [v,u,w]$ (8) $y,x,z [v,u,w]$

(9) $x+1/2,y+1/2,z [u,v,w]$ (10) $x+1/2,y+1/2,z [u,v,w]$ (11) $y,x,z [v,u,w]$ (12) $y,x,z [v,u,w]$

(13) $x,y,z [u,v,w]$ (14) $x,y,z [u,v,w]$ (15) $y+1/2,x+1/2,z [v,u,w]$ (16) $y+1/2,x+1/2,z [v,u,w]$

16 $j$ ..$m'$ $x,x+1/2,z [u,u,w]$ $x,x+1/2,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x,x+1/2,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x+1/2,x,z [u,u,w]$ $x+1/2,x,z [u,u,w]$. 

129.13.1087 - 2 - 2236
Symmetry of Special Projections

Along [0,0,1] p 4mm1'
\[ a^* = \frac{a - b}{2}, \quad b^* = \frac{a + b}{2} \]
Origin at 0,0,z

Along [1,0,0] p 2m'g'
\[ a^* = b, \quad b^* = c \]
Origin at 0,0,0

Along [1,1,0] p 22', 2mm'
\[ a^* = -c, \quad b^* = \frac{-a + b}{2} \]
Origin at x,x,1/2
Origin at \( \bar{4}/ncc \), at \(-1/4,1/4,0\) from \( \bar{1} \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

1. \( 1 \)
   
2. \( 2 \quad 0,0,z \)  
   \( (2_z|0,0,0) \)

3. \( 4^+ \quad 0,1/2,z \)  
   \( (4_z|1/2,1/2,0) \)

4. \( 4^{-} \quad 1/2,0,z \)  
   \( (4_z^{-}|1/2,1/2,0) \)

5. \( 2 \quad (0,1/2,0) \)  
   \( 1/4,y,1/4 \)  
   \( (2_y|1/2,1/2,1/2) \)

6. \( 2 \quad (1/2,0,0) \)  
   \( x,1/4,1/4 \)  
   \( (2_x|1/2,1/2,1/2) \)

7. \( 2 \quad x,x,1/4 \)  
   \( (2_x|0,0,1/2) \)

8. \( 2 \quad x,\bar{x},1/4 \)  
   \( (2_x|0,0,1/2) \)

9. \( \bar{1} \quad 1/4,1/4,0 \)  
   \( (\bar{1}|1/2,1/2,0) \)

10. \( n \quad (1/2,1/2,0) \)  
    \( x,y,0 \)  
    \( (m_x|1/2,1/2,0) \)

11. \( \bar{4}^- \quad 0,0,z; 0,0,0 \)  
    \( (4_z|0,0,0) \)

12. \( \bar{4}^- \quad 0,0,z; 0,0,0 \)  
    \( (4_z^{-}|0,0,0) \)

13. \( c \quad (0,0,1/2) \)  
    \( x,0,z \)  
    \( (m_y|0,0,1/2) \)

14. \( c \quad (0,0,1/2) \)  
    \( 0,y,z \)  
    \( (m_x|0,0,1/2) \)

15. \( c \quad (0,0,1/2) \)  
    \( x+1/2,x,z \)  
    \( (m_y|1/2,1/2,1/2) \)

16. \( n \quad (1/2,1/2,1/2) \)  
    \( x,x,z \)  
    \( (m_y|1/2,1/2,1/2) \)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
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<td>1 (1) x,y,z [u,v,w]</td>
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<td>(13) x,y,z [u,v,w]</td>
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<td>(16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p_{4mm} 4mm
\begin{align*}
a^* &= (a - b)/2 \\
b^* &= (a + b)/2
\end{align*}
Origin at 1/2,0,z

Along [1,0,0] p_{222} 2m'g'
\begin{align*}
a^* &= b \\
b^* &= c/2
\end{align*}
Origin at x,1/4,0

Along [1,1,0] p_{222} 2m'm'
\begin{align*}
a^* &= -c/2 \\
b^* &= (-a + b)/2
\end{align*}
Origin at x,x,0
Origin at $\overline{4}/ncn^1$, at $-1/4,1/4,0$ from $\overline{\overline{1}}^1$.

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For $1 +$ set

1. $1_{1}(1|0,0,0)$
   
2. $2_{2}(1|0,0,0)$

3. $4+_{3}(0,1/2,0)$
4. $4-_{4}(0,1/2,0)$

5. $2(0,1/2,0)$
6. $2(1,0,0)$

7. $2_{2}(0,0,1/2)$
8. $2_{2}(0,0,1/2)$

9. $1/4,1/4,0$
10. $n(1/2,1/2,0)$

11. $4_{4}^{+}(0,0,0)$
12. $4_{4}^{-}(0,0,0)$

13. $c(0,0,1/2)$
14. $c(0,0,1/2)$

15. $c(0,0,1/2)$
16. $c(0,0,1/2)$

$\overline{1}^1$
Continued

For 1' + set

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<th>1'</th>
<th>(1)</th>
<th>0,0,0'</th>
<th>(2)</th>
<th>2'</th>
<th>0,0,z</th>
<th>(3)</th>
<th>4'*</th>
<th>0,1/2,z</th>
<th>(4)</th>
<th>4'*</th>
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<td>(1/2,1/2,0)</td>
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<td>(12)</td>
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<td>(4')</td>
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<td>n'</td>
<td>(1/2,1/2,1/2)</td>
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<td>(14)</td>
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Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry, Coordinates

<table>
<thead>
<tr>
<th>1 +</th>
<th>1' +</th>
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<td>(15)</td>
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<td>8</td>
<td>f</td>
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<tr>
<td>(2)</td>
<td>x,y,z</td>
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**Symmetry of Special Projections**

<table>
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<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mg1'</th>
<th>Along [1,1,0]</th>
<th>p2mm1'</th>
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<tbody>
<tr>
<td>( a^* = (a - b)/2 )</td>
<td>( b^* = (a + b)/2 )</td>
<td>( a^* = b )</td>
<td>( b^* = c/2 )</td>
<td>( a^* = (-a + b)/2 )</td>
<td>( b^* = c/2 )</td>
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<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,1/4,0</td>
<td></td>
<td>Origin at x,x,0</td>
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</tbody>
</table>
Origin at $\overline{4}/n'cc$, at $-1/4,1/4,0$ from $\overline{1}'$

Asymmetric unit

$0 \leq x \leq 1/2;
0 \leq y \leq 1/2;
0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(2) 2 0,0,z
(3) $4'$ 0,1/2,z
(4) $4'\overline{1}$ 1/2,1/2,0

(5) $2'$ (0,1/2,0) 1/4,y,1/4
(6) $2'$ (1/2,0,0) x,1/4,1/4

(7) $2'$ x,x,1/4
(8) $2'$ x,x,1/4

(9) $\overline{1}$' 1/4,1/4,0
(10) $n'$ (1/2,1/2,0) x,y,0

(11) $\overline{4}'$ x,0,z; 0,0,0
(12) $\overline{4}'$ 0,0,z; 0,0,0

(13) c (0,0,1/2) x,0,z
(14) c (0,0,1/2) 0,y,z
(15) c (0,0,1/2) x+1/2,x,z

(16) n (1/2,1/2,1/2) x,x,z
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
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<td>(1) x,y,z [u,v,w]</td>
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<td>(3) y + 1/2, x + 1/2, z [v, u, w]</td>
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<td>(9) x + 1/2, y + 1/2, z [u, v, w]</td>
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<td>b</td>
<td>0, 0, 0 [0, 0, 0]</td>
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<td>1/2, 1/2, 3/4 [0, 0, w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4mm

\[ \mathbf{a}^* = \frac{\mathbf{a} - \mathbf{b}}{2} \quad \mathbf{b}^* = \frac{\mathbf{a} + \mathbf{b}}{2} \]

Origin at 0,0,z

Along [1,0,0] \( p_{2a}, 2m'g' \)

\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = c/2 \]

Origin at 1/4,1/4

Along [1,1,0] \( p_{2a}, 2m'm' \)

\[ \mathbf{a}^* = -c/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]

Origin at x,x,1/4

130.3.1090 - 2 - 2244
**Origin** at $\overline{4}'/nc'c$, at $-1/4,1/4,0$ from $1$

**Asymmetric unit**

$0 \leq x \leq 1/2; 
0 \leq y \leq 1/2; 
0 \leq z \leq 1/4$

**Symmetry Operations**

1. $1$
2. $2$ $0,0,z$
3. $4''$ $0,1/2,z$
4. $4' 
1/2,0,z$
5. $2' (0,1/2,0)$ $1/4,y,1/4$
6. $2' (1/2,0,0)$ $x,1/4,1/4$
7. $2$ $x,x,0$
8. $2$ $x,x,1/4$
9. $2''$ $1/4,1/4,0$
10. $n (1/2,1/2,0)$ $x,y,0$
11. $4'''$ $0,0,z$
12. $4'''$ $0,0,z$
13. $c' (0,0,1/2)$ $x,0,z$
14. $c' (0,0,1/2)$ $0,y,z$
15. $c (0,0,1/2)$ $x+1/2,x,z$
16. $n (1/2,1/2,1/2)$ $x,x,z$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry, Coordinates

16  g  1  (1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]
(3) y+1/2,x+1/2,z [v,u,w]  (4) y+1/2,x+1/2,z [v,u,w]
(5) x+1/2,y+1/2,z+1/2 [u,v,w]  (6) x+1/2,y+1/2,z+1/2 [u,v,w]
(7) y,x,z [v,u,w]  (8) y,x,z [v,u,w]
(9) x+1/2,y+1/2,z [v,u,w]  (10) x+1/2,y+1/2,z [v,u,w]
(11) y,x,z [v,u,w]  (12) y,x,z [v,u,w]
(13) x,y,z+1/2 [u,v,w]  (14) x,y,z+1/2 [u,v,w]
(15) y+1/2,x+1/2,z+1/2 [v,u,w]  (16) y+1/2,x+1/2,z+1/2 [v,u,w]

8  f  ..2 x,x,1/4 [u,u,0]  x,x,1/4 [u,u,0]
(1/2,1/2,0) [0,0,0,0]  (1/2,1/2,0) [0,0,0,0]
(1,2,1/2,3/4) [u,u,0]  (1,2,1/2,3/4) [u,u,0]
(1/2,0,0,0) [0,0,0,0]  (1/2,0,0,0) [0,0,0,0]

8  e  2.. 0,0,z [0,0,w]  1/2,1/2,z [0,0,w]
(1/2,1/2,0,0) [0,0,0,0]  (1/2,1/2,0,0) [0,0,0,0]
(0,0,0,0) [0,0,0,0]  (0,0,0,0) [0,0,0,0]

8  d  1 1/4,1/4,0 [u,v,w]  3/4,3/4,0 [u,v,w]
(1/4,3/4,1/2) [u,v,w]  (3/4,3,1/2) [u,v,w]
(3/4,1/4,0) [v,u,w]  (3/4,1/4,0) [v,u,w]

4  c  4'.. 0,1/2,z [0,0,0]  1/2,0,z [0,0,0]
(1/2,0,0,0) [0,0,0,0]  (1/2,0,0,0) [0,0,0,0]

4  b  2'.. 0,0,0 [0,0,0]  1/2,1/2,0 [0,0,0]
(1/2,1/2,0,0) [0,0,0,0]  (1/2,1/2,0,0) [0,0,0,0]

4  a  2.22 0,0,1/4 [0,0,0]  1/2,1/2,1/4 [0,0,0]
(1/2,1/2,3/4) [0,0,0,0]  (1/2,1/2,3/4) [0,0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p 4/m'm'  Along [1,0,0]  p 2/m'g  Along [1,1,0]  p 2/m'm'
a* = (a - b)/2  b* = (a + b)/2  a* = b  b* = c/2  a* = -c/2  b* = (-a + b)/2
Origin at 0,0,z  Origin at x,1/4,0  Origin at x,x,0
Origin at $\bar{4}'/ncn'$, at $-1/4, 1/4, 0$ from $\bar{1}$

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(1' 0,0,0)

(5) 2 (0,1/2,0) 1/4,y,1/4
(2') 1/2,1/2,1/2

(9) $\bar{1}$ 1/4,1/4,0
($\bar{1}$' 1/2,1/2,0)

(13) c (0,0,1/2) x,0,z
(m 0,0,1/2)

(2) 2 0,0,z
(2' 0,0,0)

(6) 2 (1/2,0,0) x,1/4,1/4
(2', 1/2,1/2,1/2)

(10) n (1/2,1/2,0) x,y,0
(m 1/2,1/2,0)

(11) $\bar{4}'$ 0,0,z; 0,0,0
($\bar{4}$' 0,0,0)

(14) c (0,0,1/2) 0,y,z
(m 0,0,1/2)

(15) c' (0,0,1/2) x+1/2,x,z
(m 1/2,1/2,1/2)

(16) n' (1/2,1/2,1/2) x,x,z
(m 1/2,1/2,1/2)

(3) $4'$ 0,1/2,z
($4'$ 1/2,1/2,0)

(4) $4'$ 1/2,0,z
($4'$' 1/2,1/2,0)
### Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<td></td>
<td>(3) $y+1/2,x+1/2,z$ [v,u,w]</td>
<td>(4) $y+1/2,x+1/2,z$ [v,u,w]</td>
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<td>(10) $x+1/2,y+1/2,z$ [u,v,w]</td>
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<td>(13) $x,y,z+1/2$ [u,v,w]</td>
<td>(14) $x,y,z+1/2$ [u,v,w]</td>
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<td>(15) $y+1/2,x+1/2,z+1/2$ [u,v,w]</td>
<td>(16) $y+1/2,x+1/2,z+1/2$ [v,u,w]</td>
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<td>x,x,1/4 [u,u,w]</td>
<td>x,x,1/4 [u,u,w]</td>
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<td>x+1/2,x+1/2,1/4 [u,u,w]</td>
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<td>3/4,1/4,1/2 [v,u,w]</td>
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<td>3/4,3/4,1/2 [v,u,w]</td>
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<tr>
<td>4 c 4'..</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
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<td>1/2,0,z [0,0,0]</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 b 4'..</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>4 a 2.2'2'</td>
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<td>1/2,1/2,1/4 [0,0,w]</td>
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<td>1/2,1/2,1/4 [0,0,w]</td>
<td>1/2,1/2,1/4 [0,0,w]</td>
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<td>0,0,3/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>$p_{c}$: 4mm</th>
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<tbody>
<tr>
<td>$a^* = (a - b)/2$</td>
<td>$b^* = (a + b)/2$</td>
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<tr>
<td>Origin at 0,0,z</td>
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</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>$p_{2b}$: 2m'g'</th>
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<tbody>
<tr>
<td>$a^* = b$</td>
<td>$b^* = c/2$</td>
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<td>Origin at x,1/4,0</td>
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<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>$p_{2}': mm'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = -c/2$</td>
<td>$b^* = (-a + b)/2$</td>
</tr>
<tr>
<td>Origin at x,x</td>
<td></td>
</tr>
</tbody>
</table>
Origin at \( \overline{4}n'c'n \), at \(-1/4,1/4,0\) from \( \overline{1} \)

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 4^+ \quad 0,1/2,z \\
(4) & \quad 4^+ \quad 1/2,0,z \\
(5) & \quad (2) \quad (0,1/2,0) \\
(6) & \quad (2) \quad (1/2,0,0) \\
(7) & \quad (2) \quad x,x,x \\
(8) & \quad (2) \quad x,x,x \\
(9) & \quad \overline{1} \quad 1/4,1/4,0 \\
(10) & \quad \overline{1} \quad (1/2,1/2,0) \\
(11) & \quad \overline{4}^+ \quad 0,0,z; 0,0,0 \\
(12) & \quad \overline{4}^+ \quad 0,0,z; 0,0,0 \\
(13) & \quad c' \quad (0,0,1/2) \\
(14) & \quad c' \quad (0,0,1/2) \\
(15) & \quad c \quad (0,0,1/2) \\
(16) & \quad n \quad (1/2,1/2,1/2)
\end{align*}
\]
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<tbody>
<tr>
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<td>g</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2)</td>
<td>x , y , z [u , v , w]</td>
</tr>
<tr>
<td></td>
<td>(3)</td>
<td>y + 1/2 , x + 1/2 , z [v , u , w]</td>
</tr>
<tr>
<td></td>
<td>(4)</td>
<td>x + 1/2 , y + 1/2 , z + 1/2 [u , v , w]</td>
</tr>
<tr>
<td></td>
<td>(5)</td>
<td>y , x , z + 1/2 [v , u , w]</td>
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<tr>
<td></td>
<td>(6)</td>
<td>x + 1/2 , y + 1/2 , z [u , v , w]</td>
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<td>y , x , z + 1/2 [v , u , w]</td>
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<td>y , x , z + 1/2 [v , u , w]</td>
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<tr>
<td></td>
<td>(9)</td>
<td>x + 1/2 , y + 1/2 , z [u , v , w]</td>
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<td></td>
<td>(10)</td>
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<td>x , y , z + 1/2 [u , v , w]</td>
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<td>(12)</td>
<td>x , y , z + 1/2 [u , v , w]</td>
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<td>x , y , z + 1/2 [u , v , w]</td>
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<td>(14)</td>
<td>x , y , z + 1/2 [u , v , w]</td>
</tr>
<tr>
<td></td>
<td>(15)</td>
<td>x + 1/2 , x + 1/2 , z + 1/2 [v , u , w]</td>
</tr>
<tr>
<td></td>
<td>(16)</td>
<td>x + 1/2 , x + 1/2 , z + 1/2 [v , u , w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

Along [0,0,1] p4'nm'

\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]

Origin at 0,0,z

Along [1,0,0] p2m'g'

\[ a^* = b \quad b^* = c/2 \]

Origin at x,1/4,0

Along [1,1,0] p2a'2m'm'

\[ a^* = -c/2 \quad b^* = (-a + b)/2 \]

Origin at x,x,0
Origin at $\overline{4}/n c'n'$, at $-1/4, 1/4, 0$ from $1$

Asymmetric unit $0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1 
(2) 2' 0,0,0 
(2') 0,0,0 
(3) 4' 0,1/2,0 
(4) 4' 1/2,0,0 
(5) 2' (0,1/2,0) 1/4,y,1/4 
(6) 2' (1/2,0,0) x,1/4,1/4 
(7) 2' x,x,1/4 
(8) 2' x,x,1/4 
(9) $\overline{1}$ 1/4,1/4,0 
(10) n (1/2,1/2,0) x,y,0 
(11) $\overline{4}$' 0,0,0 
(12) $\overline{4}$' 0,0,0 
(13) c' (0,0,1/2) x,0,z 
(14) c' (0,0,1/2) 0,y,z 
(15) c' (0,0,1/2) x+1/2, x,z 
(16) n' (1/2,1/2,1/2) x,x,z
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>g</td>
<td>1 (1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y+1/2,x+1/2,z [v,u,w] (4) x+1/2,y+1/2,z+1/2 [u,v,w] (5) y,x,z+1/2 [v,u,w] (6) x+1/2,y+1/2,z [u,v,w] (7) y,x,z [v,u,w] (8) x,y,z [v,u,w] (9) x,y,z [v,u,w] (10) x+1/2,y+1/2,z+1/2 [v,u,w] (11) y,x,z [v,u,w] (12) y,x,z [v,u,w] (13) x,y,z+1/2 [u,v,w] (14) x,y,z+1/2 [u,v,w] (15) y+1/2,x+1/2,z+1/2 [v,u,w] (16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>..2' x,x,1/4 [u,u,w] x,x,1/4 [u,u,w] x+1/2,x+1/2,1/4 [u,u,w] x+1/2,x+1/2,1/4 [u,u,w] x+1/2,x+1/2,3/4 [u,u,w] x+1/2,x+1/2,3/4 [u,u,w] x,x,3/4 [u,u,w] x,x,3/4 [u,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>e</td>
<td>2.. 0,0,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 0,0,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 0,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>d</td>
<td>1 1/4,1/4,0 [u,v,w] 3/4,3/4,0 [u,v,w] 3/4,3/4,0 [u,v,w] 1/4,3/4,0 [v,u,w] 1/4,3/4,0 [v,u,w] 3/4,1/4,0 [v,u,w] 3/4,1/4,0 [v,u,w]</td>
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<tr>
<td>4</td>
<td>c</td>
<td>4.. 0,1/2,z [0,0,0] 1/2,0,z+1/2 [0,0,0] 1/2,0,z+1/2 [0,0,0] 0,1/2,z+1/2 [0,0,0] 0,1/2,z+1/2 [0,0,0]</td>
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<tr>
<td>4</td>
<td>b</td>
<td>4.. 0,0,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 0,0,1/2 [0,0,0] 0,0,1/2 [0,0,0]</td>
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<tr>
<td>4</td>
<td>a</td>
<td>2.22' 0,0,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,3/4 [0,0,0] 1/2,1/2,3/4 [0,0,0] 0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p 4m'm' a* = (a - b)/2 b* = (a + b)/2
- Along [1,0,0] p 2'm'g a* = b b* = c/2
- Along [1,1,0] p2mm' a* = -c/2 b* = (-a + b)/2

Origin at 1/2,0,z Origin at x,1/4,0 Origin at x,x,0
Origin at $\overline{4}/n'cc'$, at $-1/4,1/4,0$ from $1'$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(2) 2 $0,0,z$
(3) $4'/ 0,1/2,z$
(4) $4'/ 1/2,0,z$

(5) $2' (0,1/2,0) 1/4,y,1/4$
(6) $2' (1/2,0,0) x,1/4,1/4$
(7) $2 x,x,1/4$
(8) $2 x,x,1/4$

(9) $\overline{1} 1/4,1/4,0$
(10) $n' (1/2,1/2,0) x,y,0$
(11) $4' 0,0,z; 0,0,0$
(12) $4' 0,0,z; 0,0,0$

(13) c $(0,0,1/2) x,0,z$
(14) c $(0,0,1/2) 0,y,z$
(15) $c' (0,0,1/2) x+1/2,\overline{z},z$
(16) $n' (1/2,1/2,1/2) x,x,z
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicities, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
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<td>(6) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p4'm'm
a* = (a - b)/2 b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2b* 2m'g'
a* = b b* = c/2
Origin at 1/4,1/4,0

Along [1,1,0] p2m'm'
a* = (a + b)/2 b* = c/2
Origin at x,x,0

130.8.1095 - 2 - 2254
P4/n'c'c'

130.9.1096

4/m'm'm'

P4/n'c'c'

Tetragonal

**Origin** at $\overline{4}'/n'c'n'$, at $-1/4,1/4,0$ from $\overline{1}'$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

1. $1$
   
   $1 | 0,0,0$

2. $2$ 0,0,z
   
   $2_z | 0,0,0$

3. $4^+ 0,1/2,z$
   
   $(4_z | 1/2,1/2,0)$

4. $4^- 1/2,0,z$
   
   $(4_z^{-1} | 1/2,1/2,0)$

5. $2 (0,1/2,0)$ 1/4,y,1/4
   
   $(2_y | 1/2,1/2,1/2)$

6. $2 (1/2,0,0) x,1/4,1/4$
   
   $(2_x | 1/2,1/2,1/2)$

7. $2 x,x,1/4$
   
   $(2_{xy} | 0,0,1/2)$

8. $2 x,x,1/4$
   
   $(2_{xy} | 0,0,1/2)$

9. $\overline{1}' 1/4,1/4,0$
   
   $(\overline{1} | 1/2,1/2,0)'$

10. $n' (1/2,1/2,2,0)$ x,y,0
    
    $(m_z | 1/2,1/2,2,0)'$

11. $\overline{4}' 0,0,z; 0,0,0$
    
    $(\overline{4}_z | 0,0,0)'$

12. $\overline{4}^- 0,0,z; 0,0,0$
    
    $(\overline{4}_z^{-1} | 0,0,0)'$

13. $c' (0,0,1/2) x,0,z$
    
    $(m_y | 0,0,1/2)'$

14. $c' (0,0,1/2) 0,y,z$
    
    $(m_y | 0,0,1/2)'$

15. $c' (0,0,1/2) x+1/2,x,z$
    
    $(m_{xy} | 1/2,1/2,1/2)'$

16. $n' (1/2,1/2,1/2) x,x,z$
    
    $(m_{xy} | 1/2,1/2,1/2)'$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry, Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>(14) x,y,z [v,u,w]</td>
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<td>(15) x,y,z [v,u,w]</td>
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<td>(16) x,y,z [v,u,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p4m'm'm'  
Along [1,0,0] p 2m'g'  
Along [1,1,0] p2m'm'

\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]

Origin at 0,0,z  
Origin at x,1/4,0  
Origin at x,x,0
Origin at center (mmm) at P42/mmc

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

1. 1
   (1|0,0,0)
2. 2 0,0,z
   (2z|0,0,0)
3. 4+ (0,0,1/2) 0,0,z
   (4z|0,0,1/2)
4. 4- (0,0,1/2) 0,0,z
   (4z -1|0,0,1/2)
5. 2 0,y,0
   (2y|0,0,0)
6. 2 x,0,0
   (2x|0,0,0)
7. 2 x,x,1/4
   (2xy|0,0,1/2)
8. 2 x,x,1/4
   (2xy|0,0,1/2)
9. 1 0,0,0
   (1|0,0,0)
10. m x,y,0
    (mz|0,0,0)
11. 4+ 0,0,z; 0,0,1/4
    (4z|0,0,1/2)
12. 4- 0,0,z; 0,0,1/4
    (4z -1|0,0,1/2)
13. m x,0,z
    (mz|0,0,0)
14. m 0,y,z
    (mz|0,0,0)
15. c (0,0,1/2) x,x,z
    (mxy|0,0,1/2)
16. c (0,0,1/2) x,x,z
    (mxy|0,0,1/2)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Coordinates</th>
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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
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<tr>
<td>8 p .m.</td>
<td>1/2,y,z [u,0,0]</td>
<td>1/2,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 o .m.</td>
<td>0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td>8 n ..2</td>
<td>x,x,1/4 [u,u,0]</td>
<td>x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td>4 m m2m.</td>
<td>x,1/2,0 [0,0,0]</td>
<td>x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 l m2m.</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 k m2m.</td>
<td>x,1/2,1/2 [0,0,0]</td>
<td>x,1/2,1/2 [0,0,0]</td>
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<td>4 j m2m.</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
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<tr>
<td>4 i 2mm.</td>
<td>0,1/2,z [0,0,0]</td>
<td>1/2,0,z+1/2 [0,0,0]</td>
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<td>4 h 2mm.</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
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<tr>
<td>4 g 2mm.</td>
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<td>0,0,z+1/2 [0,0,0]</td>
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<tr>
<td>2 f 4m2</td>
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<td>1/2,1/2,3/4 [0,0,0]</td>
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<tr>
<td>2 e 4m2</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
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<td>2 d mmm.</td>
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<td>0,1/2,1/2 [0,0,0]</td>
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<td>2 c mmm.</td>
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<td>0,1/2,0 [0,0,0]</td>
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<tr>
<td>2 b mmm.</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] p4mm$	ext{1}'$
\[a^* = a\qquad b^* = b\]
Origin at 0,0,z

Along [1,0,0] p2mm1'
\[a^* = b\qquad b^* = c\]
Origin at x,0,0

Along [1,1,0] p2a1$^* 2m'm'$
\[a^* = \frac{-c}{2}\qquad b^* = \frac{(-a + b)}{2}\]
Origin at x,x,0
Origin at center (mmm1') at 4/m2/mc1'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For 1 + set

(1) 1 (1 | 0,0,0)
(2) 2 0,0,z (2z | 0,0,0)
(3) 4+ (0,0,1/2) 0,0,z (4z | 0,0,1/2)
(4) 4* (0,0,1/2) 0,0,z (4z−1 | 0,0,1/2)
(5) 2 0,y,0 (2y | 0,0,0)
(6) 2 x,0,0 (2z | 0,0,0)
(7) 2 x,x,1/4 (2xy | 0,0,1/2)
(8) 2 x,x,1/4 (2xy | 0,0,1/2)
(9) 1 0,0,0 (1 | 0,0,0)
(10) m x,y,0 (mz | 0,0,0)
(11) 4+ 0,0,z; 0,0,1/4 (4z | 0,0,1/2)
(12) 4* 0,0,z; 0,0,1/4 (4z−1 | 0,0,1/2)
(13) m x,0,z (mz | 0,0,0)
(14) m 0,y,z (mz | 0,0,0)
(15) c (0,0,1/2) x,x,z (mxy | 0,0,1/2)
(16) c (0,0,1/2) x,x,z (mxy | 0,0,1/2)
Continued

For $1^+$ set

(1) $1' \ (10,0,0)$
(2) $2' \ 0,0,0 \ (2) \ 2' \ 0,0,0$
(3) $4^+ \ (0,0,1/2) \ 0,0,0 \ (4) \ 4^+ \ (0,0,1/2) \ 0,0,0$

(5) $2' \ 0,y,0 \ (2) \ 2' \ 0,y,0$
(6) $2' \ x,0,0 \ (2) \ 2' \ x,0,0$
(7) $2' \ x,x,1/4 \ (2) \ 2' \ x,x,1/4$
(8) $2' \ x,x,1/4 \ (2) \ 2' \ x,x,1/4$

(9) $1^+ \ 0,0,0 \ (1) \ 1^+ \ 0,0,0$
(10) $m' \ x,y,0 \ (2) \ m' \ x,y,0$
(11) $4^+ \ (0,0,1/4) \ 0,0,0 \ (4) \ 4^+ \ (0,0,1/4) \ 0,0,0$
(12) $4^+ \ (0,0,1/4) \ 0,0,0 \ (4) \ 4^+ \ (0,0,1/4) \ 0,0,0$

(13) $m' \ x,0,z \ (m) \ 0,0,0 \ (14) \ m' \ 0,y,0 \ (m) \ 0,0,0$
(15) $c' \ (0,0,1/2) \ x,x,1/4 \ (2) \ c' \ (0,0,1/2) \ x,x,1/4$
(16) $c' \ (0,0,1/2) \ x,x,1/4 \ (2) \ c' \ (0,0,1/2) \ x,x,1/4$

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
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<td>(4) y,x,z+1/2 [0,0,0]</td>
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<td>(5) x,y,z [0,0,0]</td>
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<td>(6) x,y,z [0,0,0]</td>
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<td>(7) y,x,z+1/2 [0,0,0]</td>
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<td>(11) y,x,z+1/2 [0,0,0]</td>
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<td>(16) y,x,z+1/2 [0,0,0]</td>
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<td>8 q m..1'</td>
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<td>x,0,0 [0,0,0]</td>
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Symmetry of Special Projections

Along [0,0,1] p4mm1'  
\[ \mathbf{a}^* = \mathbf{a}, \mathbf{b}^* = \mathbf{b} \]  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\[ \mathbf{a}^* = \mathbf{b}, \mathbf{b}^* = \mathbf{c} \]  
Origin at x,0,0

Along [1,1,0] p2mm1'  
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2, \mathbf{b}^* = \mathbf{c}/2 \]  
Origin at x,x,0
Origin at center (mmm') at 4\_2 /m'2'/mc

Asymmetric unit 
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1  (1|0,0,0)
(5) 2' 0,y,0  
(2,|0,0,0)' (2,|0,0,0)'

(9) T' 0,0,0  
(1|0,0,0)' (1|0,0,0)'

(13) m  x,0,z  
(m,|0,0,0) (m,|0,0,0)'

(2) 2 0,0,z  
(2z|0,0,0)

(6) 2' x,0,0  
(2z|0,0,0)'

(10) m' x,y,0  
(m,|0,0,0)'

(3) 4' (0,0,1/2) 0,0,z  
(4z|0,0,1/2)

(7) 2' x,x,1/4  
(2xy|0,0,1/2)'

(11) 4' 0,0,z; 0,0,1/4  
(4z|0,0,1/2)'

(4) 4' (0,0,1/2) 0,0,z  
(4z|0,0,1/2)

(8) 2' x,x,1/4  
(2xy|0,0,1/2)'

(12) 4' 0,0,z; 0,0,1/4  
(4z|0,0,1/2)'

(14) m 0,y,z  
(m,|0,0,0) (m,|0,0,0)'

(15) c (0,0,1/2) x,x,z  
(mxy|0,0,1/2) (mxy|0,0,1/2)'

(16) c (0,0,1/2) x,x,z  
(mxy|0,0,1/2) (mxy|0,0,1/2)'
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z+1/2 [v,u,w]</td>
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<td>0,0,z+1/2 [0,0,0]</td>
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<tr>
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<td>0,0,1/4 [0,0,0]</td>
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<td>0,0,1/4 [0,0,0]</td>
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<td>0,1/2,1/2 [0,0,0]</td>
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<tr>
<td>2 c m'mm.</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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<tr>
<td>2 b m'mm.</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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</tbody>
</table>
2  a  m'mmm.  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm  
\( a^* = a \)  \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\( a^* = b \)  \( b^* = c \)  
Origin at x,0,0

Along [1,1,0] p2a* 2m'm'  
\( a^* = -c/2 \)  \( b^* = (-a + b)/2 \)  
Origin at x,x,0
Origin at center (m'm'm) at $4_{2}^{'}/m2'/m'c$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $1$
   \[ (1|0,0,0) \]

2. $2' \cdot 0,0,z$
   \[ (2_{z}|0,0,0) \]

3. $4^+ \cdot (0,0,1/2) \cdot 0,0,z$
   \[ (4_{z}|0,0,1/2)' \]

4. $4^- \cdot (0,0,1/2) \cdot 0,0,z$
   \[ (4_{z}'|0,0,1/2)' \]

5. $2' \cdot 0,y,0$
   \[ (2_{y}|0,0,0)' \]

6. $2' \cdot x,0,0$
   \[ (2_{x}|0,0,0)' \]

7. $2 \cdot x,x,1/4$
   \[ (2_{xx}|0,0,1/2) \]

8. $2 \cdot x,\overline{x},1/4$
   \[ (2_{x}|0,0,1/2) \]

9. $\overline{1} \cdot 0,0,0$
   \[ (\overline{1}|0,0,0) \]

10. $m \cdot x,y,0$
    \[ (m_{x}|0,0,0) \]

11. $4\overline{2}^+ \cdot 0,0,z; 0,0,1/4$
    \[ (4_{z}|0,0,1/2)' \]

12. $4\overline{2}^- \cdot 0,0,z; 0,0,1/4$
    \[ (4_{z}'|0,0,1/2)' \]

13. $m' \cdot x,0,z$
    \[ (m_{x}|0,0,0)' \]

14. $m' \cdot 0,y,z$
    \[ (m_{y}|0,0,0)' \]

15. $c \cdot (0,0,1/2) \cdot x,\overline{x},z$
    \[ (m_{x}|0,0,1/2) \]

16. $c \cdot (0,0,1/2) \cdot x,x,z$
    \[ (m_{x}|0,0,1/2) \]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
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<tr>
<td>16 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(5) x̄,ȳ,z [ū,v̄,w]</td>
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<td>(13) x̄,ȳ,z [ū,v̄,w]</td>
</tr>
<tr>
<td>8 q m..</td>
<td>x,y,0 [0,0,w]</td>
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<tr>
<td></td>
<td>x̄,y,0 [0,0,w]</td>
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<tr>
<td>8 p .m'.</td>
<td>1/2,y,z [0,v,w]</td>
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<tr>
<td>8 n ..2</td>
<td>x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x̄,x̄,3/4 [ū,ū,0]</td>
</tr>
<tr>
<td>4 m m2m'.</td>
<td>x,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td>4 l m2m'.</td>
<td>x,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 k m2m'.</td>
<td>x,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 j m2m'.</td>
<td>x,0,0 [0,0,w]</td>
</tr>
<tr>
<td>4 i 2m'2.</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 h 2m'2.</td>
<td>1/2,1/2,z [0,0,w]</td>
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<tr>
<td>4 g 2m'2.</td>
<td>0,0,z [0,0,w]</td>
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<tr>
<td>2 f 4m'2</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
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<tr>
<td>2 e 4m'2</td>
<td>0,0,1/4 [0,0,0]</td>
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<tr>
<td>2 d mm'm'.</td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c mm'm'.</td>
<td>0,1/2,0 [0,0,w]</td>
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<td>2 b mm'm'.</td>
<td>1/2,1/2,0 [0,0,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p4mm1'  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2'mm'  
\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at x,0,0

Along [1,1,0] p2\alpha' 2m'm'  
\[ \mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]
Origin at x,x,0
P4$_1$/mmc’
131.5.1101

4’/mmm’
P4$_{1}$/m2/m2’/c’

Tetragonal

Origin at center (mmm) at 4’/m2/mc’

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
(1 0 0,0)
(1 0 0,0)

(2) 2 0,0,z
(2z 0,0,0)
(2 0,0,0)

(3) 4’+ (0,0,1/2) 0,0,z
(4z 0,0,1/2)’
(4 0,0,1/2)’

(4) 4’- (0,0,1/2) 0,0,z
(4z-1 0,0,1/2)’
(4 0,0,1/2)’

(5) 2 0,y,0
(2z 0,0,0)
(2 0,0,0)

(6) 2 x,0,0
(2z 0,0,0)
(2 0,0,0)

(7) 2’ x,x,1/4
(2xy 0,0,1/2)’
(2’ 0,0,1/2)’

(8) 2’ x,x,1/4
(2xy 0,0,1/2)’
(2’ 0,0,1/2)’

(9) 1 0,0,0
(1 0,0,0)

(10) m x,y,0
(mz 0,0,0)
(m 0,0,0)

(11) 4’+ 0,0,z; 0,0,1/4
(4z 0,0,1/2)’
(4 0,0,1/2)’

(12) 4’- 0,0,z; 0,0,1/4
(4z-1 0,0,1/2)’
(4 0,0,1/2)’

(13) m x,0,z
(mx 0,0,0)
(m 0,0,0)

(14) m 0,y,z
(mx 0,0,0)
(m 0,0,0)

(15) c’ (0,0,1/2) x,x,z
(mxy 0,0,1/2)’
(m’x 0,0,1/2)’

(16) c’ (0,0,1/2) x,x,z
(mxy 0,0,1/2)’
(m’x 0,0,1/2)’

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Generators selected \((1); t(1,0,0); t(0,1,0); t(0,0,1); \(2\); \(3\); \(5\); \(9\).

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<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
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</table>
2 a mmm. 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  
\( a^* = a \quad b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\( a^* = b \quad b^* = c \)  
Origin at x,0,0

Along [1,1,0] p2'mm'  
\( a^* = -c/2 \quad b^* = (-a + b)/2 \)  
Origin at x,x,0
Origin at center (m'm'm') at 4 symmetry operations:

1. 1
2. 2 0, 0, z
3. 4 0, 0, 1/2)
4. 4 0, 0, 1/2')
5. 2 y, 0, 0
6. 2 x, 0, 0
7. 2 x, 0, 0
8. 2 x, 0, 0
9. 1 0, 0, 0
10. 1 0, 0, 0
11. 1 0, 0, 0
12. 1 0, 0, 0
13. 1 0, 0, 0
14. 1 0, 0, 0
15. 1 0, 0, 0
16. 1 0, 0, 0

Asymmetric unit:
0 ≤ x ≤ 1/2;
0 ≤ y ≤ 1/2;
0 ≤ z ≤ 1/4

Symmetry Operations:

1. 1
2. 2 0, 0, z
3. 4 0, 0, 1/2)
4. 4 0, 0, 1/2')
5. 2 y, 0, 0
6. 2 x, 0, 0
7. 2 x, 0, 0
8. 2 x, 0, 0
9. 1 0, 0, 0
10. 1 0, 0, 0
11. 1 0, 0, 0
12. 1 0, 0, 0
13. 1 0, 0, 0
14. 1 0, 0, 0
15. 1 0, 0, 0
16. 1 0, 0, 0

Tetragonal
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>(2) x, y, z [u, v, w]</td>
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<td>8</td>
<td>q m'</td>
<td>x,y,0 [u,v,0]</td>
<td>x, y,0 [u, v, 0]</td>
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<td>p m'</td>
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<td>1/2, y, z [0, v, w]</td>
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<td>o m'</td>
<td>0,y,z [0,v,w]</td>
<td>0, y, z [0, v, w]</td>
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<td>n m'</td>
<td>x,x,1/4 [u,u,w]</td>
<td>x, x,1/4 [u, u, w]</td>
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<td>4</td>
<td>m m'2m'</td>
<td>x,1/2,0 [u,0,0]</td>
<td>x,1/2,0 [u,0,0]</td>
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<td>4</td>
<td>l m'2m'</td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
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<td>4</td>
<td>k m'2m'</td>
<td>x,1/2,1/2 [u,0,0]</td>
<td>x, 1/2,1/2 [u,0,0]</td>
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<tr>
<td>4</td>
<td>j m'2m'</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
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<tr>
<td>4</td>
<td>i 2m'</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>h 2m'</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
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<td>g 2m'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
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<td>2</td>
<td>c m'm'</td>
<td>0,1/2,0 [0,0,0]</td>
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<td>2</td>
<td>b m'm'</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</table>
2 a m'm'm'. 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4'm'm
a* = a b* = b
Origin at 0,0,z

Along [1,0,0] p2m'm'
a* = b b* = c
Origin at x,0,0

Along [1,1,0] p2a' 2m'm'
a* = -c/2 b* = (-a + b)/2
Origin at x,x,0
Origin at center (m'm'm') at $42/m2'/m'c'$

Asymmetric unit $0 < x < 1/2; \ 0 < y < 1/2; \ 0 < z < 1/4$

Symmetry Operations

1.

(1) $1$

(1|0,0,0)

(2) $2' \ 0,0,z$

($2_z|0,0,0$)

(3) $4^+ (0,0,1/2) \ 0,0,z$

($4_z|0,0,1/2$)

(4) $4^- (0,0,1/2) \ 0,0,z$

($4_z^{-1}|0,0,1/2$)

(5) $2' \ 0,y,0$

($2_y|0,0,0'$)

(6) $2' \ x,0,0$

($2_x|0,0,0'$)

(7) $2' \ x,x,1/4$

($2_{xy}|0,0,1/2'$)

(8) $2' \ x,1/2$

($2_{xy}|0,0,1/2'$)

(9) $\bar{1} \ 0,0,0$

($1|0,0,0$)

(10) $m \ x,y,0$

($m_z|0,0,0$)

(11) $4^+ \ 0,0,z; 0,0,1/4$

($4_z|0,0,1/2$)

(12) $4^- \ 0,0,z; 0,0,1/4$

($4_z^{-1}|0,0,1/2$)

(13) $m' \ x,0,z$

($m_z|0,0,0'$)

(14) $m' \ 0,y,z$

($m_z|0,0,0'$)

(15) $c' (0,0,1/2) \ x,\bar{x},z$

($m_{xy}|0,0,1/2'$)

(16) $c' (0,0,1/2) \ x,\bar{x},z$

($m_{xy}|0,0,1/2'$)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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<th>Coordinates</th>
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</table>
Symmetry of Special Projections

Along [0,0,1] p4mm1'

\( a^* = a \quad b^* = b \)

Origin at 0,0,z

Along [1,0,0] p2'mm'

\( a^* = -c \quad b^* = b \)

Origin at x,0,0

Along [1,1,0] p 2'mm'

\( a^* = -c/2 \quad b^* = (-a + b)/2 \)

Origin at x,x,0
**Origin** at center (mmm') at 42'/m2'/mc'

**Asymmetric unit** \[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\]

**Symmetry Operations**

(1) \(1\) \((1|0,0,0)\)

(2) \(2\) \((0,0,z)\)
\((2_z|0,0,0)\)

(3) \(4^{+} (0,0,1/2)\) \((0,0,z)\)
\((4_z|0,0,1/2)\)

(4) \(4^{-} (0,0,1/2)\) \((0,0,z)\)
\((4_z^{-1}|0,0,1/2)\)

(5) \(2'\) \((0,y,0)\)
\((2_y|0,0,0)\)

(6) \(2'\) \((x,0,0)\)
\((2_x|0,0,0)\)

(7) \(2\) \((x,x,1/4)\)
\((2_{xy}|0,0,1/2)\)

(8) \(2\) \((x,x,1/4)\)
\((2_{xy}|0,0,1/2)\)

(9) \(T'\) \((0,0,0)\)
\((1|0,0,0)\)

(10) \(m'\) \((x,y,0)\)
\((m_x|0,0,0)\)

(11) \(4^{+}\) \((0,0,z; 0,0,1/4)\)
\((4_z|0,0,1/2)\)

(12) \(4^{-}\) \((0,0,z; 0,0,1/4)\)
\((4_z^{-1}|0,0,1/2)\)

(13) \(m\) \((x,0,z)\)
\((m_x|0,0,0)\)

(14) \(m\) \((0,y,z)\)
\((m_y|0,0,0)\)

(15) \(c'\) \((0,0,1/2)\) \((x,x,z)\)
\((m_{xy}|0,0,1/2)\)

(16) \(c'\) \((0,0,1/2)\) \((x,x,z)\)
\((m_{xy}|0,0,1/2)\)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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<td>(1) x,y,z [u,v,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p4'mm'  
\(a^* = a\quad b^* = b\)  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\(a^* = b\quad b^* = c\)  
Origin at x,0,0

Along [1,1,0] p2m'm'  
\(a^* = (a + b)/2\quad b^* = c/2\)  
Origin at x,x,0
Origin at center (m'm'm') at 4/m'2/m'c'

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

1. \(1\) (1|0,0,0)
2. \(2\) \(0,0,z\) \(0,0,0\)
3. \(4^+\) \((0,0,1/2)\) \((0,0,0)\)
4. \(4^-\) \((0,0,1/2)\) \((0,0,1/2)\)
5. \(2\) \(0,y,0\) \(2_x,0,0\)
6. \(2\) \(x,0,0\) \(2_x,0,0\)
7. \(2\) \(x,x,1/4\) \(2_{xy},0,0\)
8. \(2\) \(x,x,1/4\) \(2_{xy},0,0\)
9. \(\bar{1}\) \(0,0,0\) \(2_y,0,0\)
10. \(m'\) \(x,y,0\) \(m_x,0,0\)
11. \(\bar{4}^{+}\) \(0,0,z\) \(0,0,1/2\)
12. \(\bar{4}^{-}\) \(0,0,z\) \(0,0,1/2\)
13. \(m'\) \(x,0,z\) \(m_x,0,0\)
14. \(m'\) \(y,z\) \(m_y,0,0\)
15. \(c'\) \((0,0,1/2)\) \(x,x,z\) \(m_{xy},0,0\)
16. \(c'\) \((0,0,1/2)\) \(x,x,z\) \(m_{xy},0,0\)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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2  a  m'm'm'.  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4m'm'
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p2m'm'
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p2m'm'
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
**Origin** at center (mmm) at $P_{4}2/mc$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

For $(0,0,0) + \text{ set}$

1. $1$
   
   $(1|0,0,0)$

2. $2\overline{1}$
   
   $(0,0,z)$

3. $4\overline{1}$
   
   $(0,0,1/2)$

4. $4\overline{1}$
   
   $(0,0,1/2)$

5. $2$
   
   $(0,y,0)$

6. $2$
   
   $(x,0,0)$

7. $2$
   
   $(x,x,1/4)$

8. $2$
   
   $(x,x,1/4)$

9. $m$
   
   $(x,z)$

10. $m$
    
    $(0,y,0)$

11. $4$
    
    $(0,0,z; 0,0,1/4)$

12. $4$
    
    $(0,0,z; 0,0,1/4)$

13. $m$
    
    $(x,0,z)$

14. $m$
    
    $(0,y,z)$

15. $c$
    
    $(0,0,1/2)$

16. $c$
    
    $(0,0,1/2)$
## Positions

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<td>x,1/2,0 [0,0,w]</td>
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<td></td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>8 l m2m.</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
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<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8 k m2'.</td>
<td>x,1/2,1/2 [0,0,w]</td>
<td>x,1/2,1/2 [0,0,w]</td>
<td>x,1/2,1/2 [0,0,w]</td>
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<tr>
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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>8 j m2m.</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
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<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>8 i 2'm'.</td>
<td>0,1/2,z [u,0,0]</td>
<td>0,1/2,z [u,0,0]</td>
<td>0,1/2,z [u,0,0]</td>
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<tr>
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<td></td>
<td>(1) x,y,z [u,v,w]</td>
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</table>

For (1,0,0)' + set

(1) t' (1,0,0)  (2) 2' 1/2,0,z  (3) 4' (0,0,1/2) 1/2,1/2,z  (4) 4' (0,0,1/2) 1/2,-1/2,z  (5) 2' 1/2,y,0  (6) 2' (1,0,0) x,0,0  (7) 2' (1/2,1/2,0) x+1/2,x,1/4  (8) 2' (1/2,-1/2,0) x+1/2,x,1/4  (9) 1' 1/2,0,0  (10) a' (1,0,0) x,y,0  (11) 4' 1/2,-1/2,1/2 1/2,-1/2,1/4  (12) 4' 1/2,1/2,1/2 1/2,1/2,1/4  (13) a' (1,0,0) x,0,z  (14) m' 1/2,y,z  (15) n' (1/2,1/2,1/2) x+1/2,x,z  (16) n' (1/2,1/2,1/2) x+1/2,x,z

---

**Generators selected**

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).
<p>| | | | | | |</p>
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<td>0,0,0+z/2 [0,0,0]</td>
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<td>4</td>
<td>f</td>
<td>mm'2</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>mm'2</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>mmm'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>mmm'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>mmm'</td>
<td>1/2,1/2,0 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
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<tr>
<td>4</td>
<td>a</td>
<td>mmm</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
**\( a^* = a \)  \( b^* = b \)**

Origin at 0,0,z

Along [1,0,0] p2mm1'  
**\( a^* = b \)  \( b^* = c \)**

Origin at x,0,0

Along [1,1,0] p_4\textsuperscript{2}mm  
**\( a^* = (a + b)/2 \)  \( b^* = c/2 \)**

Origin at x-1/4,x+1/4,0
Origin at center (mmm') at 42/m2'mc

Asymmetric unit 
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(5) 2' 0,y,0
(2y|0,0,0)'

(9) 1' 0,0,0
(1|0,0,0)'

(13) m  x,0,z
(m|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(6) 2' x,0,0
(2x|0,0,0)'

(10) m' x,y,0
(mz|0,0,0)'

(3) 4' (0,0,1/2) 0,0,z
(4z|0,0,1/2)

(7) 2' x,x,1/4
(2xy|0,0,1/2)'

(11) 4' (0,0,1/2) 0,0,z
(4z|0,0,1/2)

(8) 2' x,x,1/4
(2xy|0,0,1/2)'

(12) 4' (0,0,1/2) 0,0,z
(4z|0,0,1/2)

(14) m 0,y,z
(mx|0,0,0)


Continued

For \((1,0,0)\)' + set

\[
\begin{align*}
(1) \ t'(1,0,0) & \quad (2) \ 2' \ 1/2,0,z \\
(2,1,0,0)' & \quad (3) \ 4' \ (0,0,1/2) \ 1/2,1/2,z \\
(2,1,0,0)' & \quad (4) \ 4' \ (0,0,1/2) \ 1/2,-1/2,z \\
\end{align*}
\]

\[
\begin{align*}
(5) \ 2 & \ 1/2,y,0 \\
(2,1,0,0)' & \quad (6) \ 2 \ (1,0,0) \ x,0,0 \\
(2,1,0,0)' & \quad (7) \ 2 \ (1/2,1/2,0) \ x+1/2,x,1/4 \\
(2,1,0,0)' & \quad (8) \ 2 \ (1/2,1/2,0) \ x+1/2,x,1/4 \\
\end{align*}
\]

\[
\begin{align*}
(9) \ 1/2,2,0,0 & \quad (10) \ a \ (1,0,0) \ x,y,0 \\
(1,0,0)' & \quad (11) \ 4' \ 1/2,1/2,0; \ 1/2,-1/2,1/4 \\
(1,0,0)' & \quad (12) \ 4' \ 1/2,1/2,0; \ 1/2,-1/2,1/4 \\
\end{align*}
\]

\[
\begin{align*}
(13) \ a'(1,0,0) & \quad (14) \ m' \ 1/2,y,z \\
(3,1,0,0)' & \quad (15) \ n' \ (1/2,1/2,1/2) \\
(3,1,0,0)' & \quad (16) \ n' \ (1/2,1/2,1/2) \\
\end{align*}
\]

\[
\begin{align*}
(13) \ a'(1,0,0) & \quad (14) \ m' \ 1/2,y,z \\
(3,1,0,0)' & \quad (15) \ n' \ (1/2,1/2,1/2) \\
(3,1,0,0)' & \quad (16) \ n' \ (1/2,1/2,1/2) \\
\end{align*}
\]

Generators selected

(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>((0,0,0) + (1,0,0)' + )</td>
</tr>
<tr>
<td>32 \ r \ 1</td>
<td>(1) \ x,y,z \ [u,v,w] \ (2) \ x, y, z \ [u, v, w] \ (3) \ y, x, z+1/2 \ [v, u, w] \ (4) \ y, x, z+1/2 \ [v, u, w]</td>
</tr>
<tr>
<td>16 \ q \ dotted \ m'.</td>
<td>x,0 \ [u, v, 0] \ x,0 \ [u, v, 0] \ y, x, 1/2 \ [v, u, 0] \ y, x, 1/2 \ [v, u, 0]</td>
</tr>
<tr>
<td>16 \ p \ dotted \ m'.</td>
<td>1/2, y, z \ [0, v, w] \ y, 1/2, z+1/2 \ [v, 0, w] \ y, 1/2, z+1/2 \ [v, 0, w]</td>
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<tr>
<td>16 \ o \ m.</td>
<td>0, y, z \ [u, 0, 0] \ 0, y, z \ [u, 0, 0] \ y, 0, z+1/2 \ [0, u, 0] \ y, 0, z+1/2 \ [0, u, 0]</td>
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<tr>
<td>16 \ n \ dotted' \ 2'</td>
<td>x, x, 1/2 \ [u, u, w] \ x, x, 1/2 \ [u, u, w] \ x, x, 3/2 \ [u, u, w] \ x, x, 3/2 \ [u, u, w]</td>
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<tr>
<td>8 \ m \ m'2m'.</td>
<td>x, 1/2, 0 \ [u, 0, 0] \ x, 1/2, 0 \ [u, 0, 0] \ 1/2, x, 1/2 \ [0, u, 0] \ 1/2, x, 1/2 \ [0, u, 0]</td>
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<td>8 \ l \ m'2m'.</td>
<td>x, 0, 1/2 \ [0, v, 0] \ 0, x, 1/2 \ [0, v, 0] \ 0, x, 0 \ [v, 0, 0]</td>
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<tr>
<td>8 \ k \ m'2m'.</td>
<td>x, 1/2, 1/2 \ [u, 0, 0] \ x, 1/2, 1/2 \ [u, 0, 0] \ 1/2, x, 0 \ [0, u, 0] \ 1/2, x, 0 \ [0, u, 0]</td>
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<tr>
<td>8 \ j \ m'2m'.</td>
<td>x, 0, 0 \ [0, v, 0] \ 0, x, 1/2 \ [v, 0, 0] \ 0, x, 1/2 \ [v, 0, 0]</td>
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<td>0, 1/2, z \ [u, 0, 0] \ 0, 1/2, z \ [u, 0, 0] \ 1/2, 0, z+1/2 \ [0, u, 0] \ 1/2, 0, z+1/2 \ [0, u, 0]</td>
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### Symmetry of Special Projections

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<td>0,0,z [0,0,0]</td>
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<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
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<tr>
<td>4</td>
<td>f</td>
<td>(\bar{4}m'2')</td>
<td>1/2,1/2,1/4 [0,0,w]</td>
<td>1/2,1/2,3/4 [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>(\bar{4}m2')</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>m'm'm'.</td>
<td>0,1/2,1/2 [u,0,0]</td>
<td>1/2,0,0 [0,u,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>m'mm'.</td>
<td>0,1/2,0 [u,0,0]</td>
<td>1/2,0,1/2 [0,u,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>m'm'm'.</td>
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<td></td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>m'mm.</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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Along [0,0,1] \(p_0.4mm\)

\[a^* = a \quad b^* = b\]

Origin at 0,0,z

Along [1,0,0] \(p2mm1'\)

\[a^* = b \quad b^* = c\]

Origin at x,0,0

Along [1,1,0] \(p_0.2m'm'\)

\[a^* = (-a + b)/2 \quad b^* = c/2\]

Origin at x,x,0

---

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Origin at center (m'm'm) at \(4_2/m2'/m'c'\)

Asymmetric unit
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4\]

Symmetry Operations
For \((0,0,0) + \) set

1. \[1 \quad (1|0,0,0)\]
2. \[2' \quad 0,0,z \quad (2_z|0,0,0)\]
3. \[4^+ (0,0,1/2) \quad 0,0,z \quad (4_z|0,0,1/2)\]
4. \[4^- (0,0,1/2) \quad 0,0,z \quad (4_z^{-1}|0,0,1/2)\]
5. \[2' \quad 0,y,0 \quad (2_y|0,0,0)\]
6. \[2' \quad x,0,0 \quad (2_x|0,0,0)\]
7. \[2' \quad x,x,1/4 \quad (2_{xy}|0,0,1/2)\]
8. \[2' \quad x,x,1/4 \quad (2_{xy}^{-1}|0,0,1/2)\]
9. \[1 \quad 0,0,0 \quad (1|0,0,0)\]
10. \[m \quad x,y,0 \quad (m_x|0,0,0)\]
11. \[4^+ (0,0,1/4) \quad 0,0,1/4 \quad (4_z|0,0,1/2)\]
12. \[4^- (0,0,1/4) \quad 0,0,1/4 \quad (4_z^{-1}|0,0,1/2)\]
13. \[m' \quad x,0,z \quad (m_x|0,0,0)\]
14. \[m' \quad 0,y,z \quad (m_y|0,0,0)\]
15. \[c' \quad (0,0,1/2) \quad x,x,z \quad (m_{xy}|0,0,1/2)\]
16. \[c' \quad (0,0,1/2) \quad x,x,z \quad (m_{xy}|0,0,1/2)\]
For \((1,0,0)' + \) set

| (1) \(t'(1,0,0)\) | (2) \(2'(1/2,0,z)\) & (3) \(4'^+ (0,0,1/2)\) & (4) \(4'^- (0,0,1/2)\) |
|-----------------|-----------------|-----------------|-----------------|
| \((1|0,0)'\)    | \((2|1,0,0)'\) & \((4|1,0,1/2)'\) & \((4|1,0,1/2)'\) |

| (5) \(2|1/2,y,0\) & (6) \(2|1,0,0)\) & (7) \(2|1/2,1/2,0\) & (8) \(2|1/2,1/2,0\) |
|-----------------|-----------------|-----------------|-----------------|
| \((2|1,0,0)\) & \((2|1,0,0)\) & \((2|1,0,1/2)\) & \((2|1,0,1/2)\) |

| (9) \(T(1/2,0,0)'\) & (10) \(a'(1,0,0)\) & (11) \(\bar{4}'\) & (12) \(\bar{4}'\) |
|-----------------|-----------------|-----------------|-----------------|
| \((m|1,0,0)'\) & \((m|x,1/2,0)\) & \((4|x,1/2,1/2)'\) & \((4|x,1/2,1/2)'\) |

| (13) \(a|1,0,0)\) & (14) \(m|1/2,y,z\) & (15) \(n|1/2,-1/2,1/2\) & (16) \(n|1/2,1/2,1/2\) |
|-----------------|-----------------|-----------------|-----------------|
| \((m|x,1/2,0)\) & \((m|x,y,0)\) & \((m|x,1/2,0)\) & \((m|x,1/2,0)\) |

Generators selected \((1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<th>Site Symmetry</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>32 r 1</td>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
<td>(0,0,0) + (1,0,0)' +</td>
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<tr>
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<td>(2) (\bar{x},\bar{y},z)</td>
<td>[(\bar{u},\bar{v},w)]</td>
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<td>(3) (y,x,z+1/2)</td>
<td>[(\bar{v},u,w)]</td>
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<td></td>
<td>(4) (y,x,z+1/2)</td>
<td>[(v,u,w)]</td>
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<tr>
<td></td>
<td>(5) (\bar{x},\bar{y},z)</td>
<td>[(u,v,w)]</td>
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<td>(6) (\bar{x},\bar{y},z)</td>
<td>[(u,v,w)]</td>
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<td></td>
<td>(7) (y,x,z+1/2)</td>
<td>[(\bar{v},u,w)]</td>
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<td>(8) (y,x,z+1/2)</td>
<td>[(v,u,w)]</td>
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<td>(9) (\bar{x},\bar{y},z)</td>
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<td>[(\bar{v},u,w)]</td>
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<td>(15) (y,x,z+1/2)</td>
<td>[(\bar{v},u,w)]</td>
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<td>(16) (y,x,z+1/2)</td>
<td>[(v,u,w)]</td>
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</table>

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<tr>
<th>16 q m..</th>
<th>x,y,0 [0,0,0]</th>
<th>(\bar{x},\bar{y},0) [0,0,0]</th>
<th>(y,x,1/2) [0,0,0]</th>
<th>(y,x,1/2) [0,0,0]</th>
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<tbody>
<tr>
<td>16 p .m.</td>
<td>1/2,y,z [u,0,0]</td>
<td>1/2,(\bar{y},z) [u,0,0]</td>
<td>(\bar{y},1/2,z+1/2) [0,u,0]</td>
<td>(y,1/2,z+1/2) [0,u,0]</td>
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<tr>
<td>16 o .m'</td>
<td>0,y,z [0,v,w]</td>
<td>0,(\bar{y},z) [0,v,w]</td>
<td>(\bar{y},0,z+1/2) [v,0,w]</td>
<td>(y,0,z+1/2) [v,0,w]</td>
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<tr>
<td>16 n ..2'</td>
<td>x,x,1/4 [u,u,w]</td>
<td>(\bar{x},\bar{x},1/4) [u,u,w]</td>
<td>(\bar{x},3/4) [u,u,w]</td>
<td>(x,3/4) [u,u,w]</td>
</tr>
<tr>
<td>8 m m2m.</td>
<td>x,1/2,0 [0,0,0]</td>
<td>(\bar{x},1/2,0) [0,0,0]</td>
<td>1/2,x,1/2 [0,0,0]</td>
<td>1/2,(\bar{x},1/2) [0,0,0]</td>
</tr>
<tr>
<td>8 l m2'm.</td>
<td>x,0,1/2 [0,0,0]</td>
<td>(\bar{x},0,1/2) [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
<td>0,(\bar{x},0) [0,0,0]</td>
</tr>
</tbody>
</table>

### Coordinates

- \((0,0,0)\) + \((1,0,0)' + \)
- \((1) x,y,z\) \([u,v,w]\)
- \((2) \bar{x},\bar{y},z\) \([\bar{u},\bar{v},w]\)
- \((3) y,x,z+1/2\) \([\bar{v},u,w]\)
- \((4) y,x,z+1/2\) \([v,u,w]\)
- \((5) \bar{x},\bar{y},z\) \([u,v,w]\)
- \((6) \bar{x},\bar{y},z\) \([u,v,w]\)
- \((7) y,x,z+1/2\) \([\bar{v},u,w]\)
- \((8) y,x,z+1/2\) \([v,u,w]\)
- \((9) \bar{x},\bar{y},z\) \([u,v,w]\)
- \((10) \bar{x},\bar{y},z\) \([u,v,w]\)
- \((11) y,x,z+1/2\) \([\bar{v},u,w]\)
- \((12) y,x,z+1/2\) \([v,u,w]\)
- \((13) \bar{x},\bar{y},z\) \([u,v,w]\)
- \((14) \bar{x},\bar{y},z\) \([u,v,w]\)
- \((15) y,x,z+1/2\) \([\bar{v},u,w]\)
- \((16) y,x,z+1/2\) \([v,u,w]\)

Continued
### Symmetry of Special Projections

<table>
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<tr>
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<th>Kaleidoscopic Generation</th>
<th>Mother Space Group</th>
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<tr>
<td>8</td>
<td>h</td>
<td>2mm.</td>
<td>Along [0,0,1]</td>
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<td></td>
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<td>1/2,1/2,z [0,0,0]</td>
<td>p4mm1'</td>
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<td>1/2,1/2,z+1/2 [0,0,0]</td>
<td>p2mm1'</td>
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<tr>
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<td>1/2,1/2,z+1/2 [0,0,0]</td>
<td>p2a 2mm</td>
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<tr>
<td>8</td>
<td>g</td>
<td>2m'2'</td>
<td>Along [1,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>0,0,z [0,0,w]</td>
<td>b* = c</td>
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<td>0,0,z+1/2 [0,0,w]</td>
<td>a* = (-a + b)/2</td>
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<td>0,0,0 [0,0,w]</td>
<td>Origin at x,0,0</td>
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<td>1/2,1/2,3/4 [0,0,0]</td>
<td>p2a 2mm</td>
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<td>0,0,1/4 [0,0,w]</td>
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<td>0,0,1/2 [0,0,w]</td>
<td>p2a 2mm</td>
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</tbody>
</table>
Origin at center (mmm') at 42'/m'2'/mc'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1'0,0,0)

(2) 2 0,0,z
(2z0,0,0)

(3) 4' (0,0,1/2) 0,0,z
(4z0,0,1/2')

(4) 4' (0,0,1/2) 0,0,z
(4z0,0,1/2')

(5) 2' y,y,0
(2y0,0,0)

(6) 2' x,0,0
(2x0,0,0')

(7) 2 x,0,1/4
(2x0,0,1/2)

(8) 2 x,x,1/4
(2y0,0,1/2)

(9) T' 0,0,0
(1'0,0,0')

(10) m' x,y,0
(mz0,0,0')

(11) 4' 0,0,z; 0,0,1/4
(4z0,0,1/2)

(12) 4' 0,0,z; 0,0,1/4
(4z0,0,1/2')

(13) m x,0,z
(mz0,0,0)

(14) m 0,y,z
(mx0,0,0)

(15) c' (0,0,1/2) x,x,z
(mx0,0,1/2')

(16) c' (0,0,1/2) x,x,z
(mx0,0,1/2')
For (1,0,0)' + set

Continued

Generators selected
(1); t'(1,0,0); t'((0,1,0)); t(0,0,1); (2); (3); (5); (9).

Positions

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<td>(1,0,0)' +</td>
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<tr>
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<td>0,x,1/4 [u,u,0]</td>
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<td>x,1/2,0 [u,0,0]</td>
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<td>x,1/2,0 [u,0,0]</td>
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<td>1/2,x,1/2 [0,u,0]</td>
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<td>1/2,x,1/2 [0,u,0]</td>
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<tr>
<td>8 k m'2m'.</td>
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<td>8 j m'2m'.</td>
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<tr>
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</tr>
<tr>
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<td>0,1/2,z [u,0,0]</td>
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</tr>
<tr>
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<td>1/2,0,z+1/2 [0,u,0]</td>
</tr>
</tbody>
</table>

Wyckoff point

-1 31.13.1109 - 2 - 2294
| 8  | h  | 2m'h'. | 1/2,1/2,z [0,0,w] | 1/2,1/2,z+1/2 [0,0,w] | 1/2,1/2,z [0,0,w] | 1/2,1/2,z+1/2 [0,0,w] |
| 8  | g  | 2mm.   | 0,0,z [0,0,0]     | 0,0,z+1/2 [0,0,0]     | 0,0,z [0,0,0]     | 0,0,z+1/2 [0,0,0]     |
| 4  | f  | 4'm'2  | 1/2,1/2,1/4 [0,0,0] | 1/2,1/2,3/4 [0,0,0] | 1/2,1/2,1/4 [0,0,0] | 1/2,1/2,3/4 [0,0,0] |
| 4  | e  | 4'm2   | 0,0,1/4 [0,0,0]    | 0,0,3/4 [0,0,0]       | 0,0,1/4 [0,0,0]    | 0,0,3/4 [0,0,0]       |
| 4  | d  | m'm'm'. | 0,1/2,1/2 [0,v,0]  | 1/2,0,0 [v,0,0]       | 0,1/2,1/2 [0,v,0]  | 1/2,0,0 [v,0,0]       |
| 4  | c  | m'm'm'. | 0,1/2,0 [0,v,0]    | 1/2,0,1/2 [v,0,0]     | 0,1/2,0 [0,v,0]    | 1/2,0,1/2 [v,0,0]     |
| 4  | b  | m'm'm'. | 1/2,1/2,0 [0,0,0]  | 1/2,1/2,1/2 [0,0,0]   | 1/2,1/2,0 [0,0,0]  | 1/2,1/2,1/2 [0,0,0]   |
| 4  | a  | m'm'm. | 0,0,0 [0,0,0]      | 0,0,1/2 [0,0,0]       | 0,0,0 [0,0,0]      | 0,0,1/2 [0,0,0]       |

**Symmetry of Special Projections**

Along [0,0,1] p_{4'} 4m'm'

\[ a^* = a \quad b^* = b \]

Origin at 1/2,1/2,z

Along [1,0,0] p2mm1'

\[ a^* = b \quad b^* = c \]

Origin at x,0,0

Along [1,1,0] p_{2x} 2m'm'

\[ a^* = (-a + b)/2 \quad b^* = c/2 \]

Origin at x,x,0
Origin at center (mmm) at $4/m/mc2/m$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \geq y$

Symmetry Operations

1. $1$
   - $(1|0,0,0)$

2. $2$
   - $(2|0,0,z)$
   - $(2|z,0,0,0)$

3. $4^+$
   - $(0,0,1/2)\ 0,0,z$
   - $(4|z,0,0,1/2)$

4. $4^-$
   - $(0,0,1/2)\ 0,0,z$
   - $(4|z^{-1},0,0,1/2)$

5. $2$
   - $0, y, 1/4$
   - $(2|0,0,1/2)$

6. $2$
   - $x, 0, 1/4$
   - $(2|z,0,0,1/2)$

7. $2$
   - $x, x, 0$
   - $(2|x,0,0,0)$

8. $2$
   - $x, x, 0$
   - $(2|x,0,0,0)$

9. $T$
   - $0, 0, 0$
   - $(1|0,0,0)$

10. $m$
    - $x, y, 0$
    - $(m|x,0,0,0)$

11. $4^+$
    - $0, 0, z;\ 0, 0, 1/4$
    - $(4|z,0,0,1/2)$

12. $4^-$
    - $0, 0, z;\ 0, 0, 1/4$
    - $(4|z^{-1},0,0,1/2)$

13. $c$
    - $(0,0,1/2)\ x, 0, z$
    - $(m|x,0,0,1/2)$

14. $c$
    - $(0,0,1/2)\ 0, y, z$
    - $(m|x,0,0,1/2)$

15. $m$
    - $x, \bar{x}, z$
    - $(m|x,0,0,0)$

16. $m$
    - $x, x, z$
    - $(m|x,0,0,0)$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
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<th>Wyckoff letter</th>
<th>Coordinates</th>
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<td>x,x,z+1/2 [u,u,0]</td>
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132.1.1110 - 2 - 2297
Symmetry of Special Projections

Along [0,0,1] p4mm1'
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2a* 2m'm'
\[ \mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = \mathbf{b} \]
Origin at x,0,1/4

Along [1,1,0] p2mm1'
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,0
**Origin** at center (mmm1') at 4/m/mc2/m1'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y \]

**Symmetry Operations**

For 1 + set

1. \((1) 1 (1|0,0,0)\)
2. \((2) 2 (0,0,z) (2_z|0,0,0)\)
3. \((3) 4^+ (0,0,1/2) 0,0,z (4_z|0,0,1/2)\)
4. \((4) 4^- (0,0,1/2) 0,0,z (4_z^{-1}|0,0,1/2)\)
5. \((5) 2 0,y,1/4 (2_y|0,0,1/2)\)
6. \((6) 2 x,0,1/4 (2_x|0,0,1/2)\)
7. \((7) 2 x,x,0 (2_{xy}|0,0,0)\)
8. \((8) 2 x,x,0 (2_{xy}|0,0,0)\)
9. \((9) \overline{1} 0,0,0 (1|0,0,0)\)
10. \((10) m x,y,0 (m_x|0,0,0)\)
11. \((11) \overline{4}^+ 0,0,z; 0,0,1/4 (4_z|0,0,1/2)\)
12. \((12) \overline{4}^- 0,0,z; 0,0,1/4 (4_z^{-1}|0,0,1/2)\)
13. \((13) c (0,0,1/2) x,0,z (m_y|0,0,1/2)\)
14. \((14) c (0,0,1/2) 0,y,z (m_x|0,0,1/2)\)
15. \((15) m x,x,z (m_{xy}|0,0,0)\)
16. \((16) m x,x,z (m_{xy}|0,0,0)\)
Continued

### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

### Positions

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**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  
Origin at 0,0,z

Along [1,0,0] p 2mm1'  
\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}/2 \]  
Origin at x,0,0

Along [1,1,0] p2mm1'  
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]  
Origin at x,x,0
**P4₂/m'cm**  
132.3.1112

**4/m'mm**  
P4₂/m'2'/c2'/m  
Tetragonal

**Origin** at center (mmm') at 4₂/m'c2'/m

**Asymmetric unit**  
0 ≤ x ≤ 1/2;  
0 ≤ y ≤ 1/2;  
0 ≤ z ≤ 1/2;  
x ≤ y

**Symmetry Operations**

1.  
   \( \begin{align*}  
   \bar{1} & \quad (x, y, 0) \\
   \end{align*} \)

2.  
   \( \begin{align*}  
   2 & \quad (0, 0, z) \\
   (2z, 0, 0, 0) \\
   \end{align*} \)

3.  
   \( \begin{align*}  
   4' & \quad (0, 0, 1/2) \\
   0, 0, z \\
   (4z, 0, 0, 1/2) \\
   \end{align*} \)

4.  
   \( \begin{align*}  
   4' & \quad (0, 0, 1/2) \\
   0, 0, z \\
   (4z, 0, 0, 1/2) \\
   \end{align*} \)

5.  
   \( \begin{align*}  
   2' & \quad 0, y, 1/4 \\
   (2y, 0, 0, 1/2)' \\
   \end{align*} \)

6.  
   \( \begin{align*}  
   2' & \quad x, 0, 1/4 \\
   (2z, 0, 0, 1/2)' \\
   \end{align*} \)

7.  
   \( \begin{align*}  
   2' & \quad x, x, 0 \\
   (2x, 0, 0, 0)' \\
   \end{align*} \)

8.  
   \( \begin{align*}  
   2' & \quad x, x, 0 \\
   (2x, 0, 0, 0)' \\
   \end{align*} \)

9.  
   \( \begin{align*}  
   \bar{1}' & \quad 0, 0, 0 \\
   (1, 0, 0, 0)' \\
   \end{align*} \)

10.  
    \( \begin{align*}  
    m' & \quad x, y, 0 \\
    (mz, 0, 0, 0)' \\
    \end{align*} \)

11.  
    \( \begin{align*}  
    \bar{4} & \quad 0, 0, z; 0, 0, 1/4 \\
    (4z, 0, 0, 1/2)' \\
    \end{align*} \)

12.  
    \( \begin{align*}  
    \bar{4} & \quad 0, 0, z; 0, 0, 1/4 \\
    (4z, 0, 0, 1/2)' \\
    \end{align*} \)

13.  
    \( \begin{align*}  
    c & \quad (0, 0, 1/2) \\
    x, 0, z \\
    (m, 0, 0, 1/2) \\
    \end{align*} \)

14.  
    \( \begin{align*}  
    c & \quad (0, 0, 1/2) \\
    0, y, z \\
    (m, 0, 0, 1/2) \\
    \end{align*} \)

15.  
    \( \begin{align*}  
    m & \quad x, x, z \\
    (m, 0, 0, 0) \\
    \end{align*} \)

16.  
    \( \begin{align*}  
    m & \quad x, x, z \\
    (m, 0, 0, 0) \\
    \end{align*} \)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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Symmetry of Special Projections

Along [0,0,1]  p4mm
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0]  p_{2a'*2m'm'}
\[ \mathbf{a}^* = -\frac{c}{2} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at x,0,0

Along [1,1,0]  p2mm1'
\[ \mathbf{a}^* = -\frac{\mathbf{a} + \mathbf{b}}{2} \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,0
**Origin** at center (mmm) at 4'/mc'm

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y\]

**Symmetry Operations**

(1) 1
(1) 1
(5) 2' 0,y,1/4

(2) 2 0,0,z

(6) 2' x,0,1/4

(7) 2 x,x,0

(8) 2 x,x,0

(9) \(\overline{1}\) 0,0,0

(10) m x,y,0

(11) 4' \((0,0,1/2), 0,0,z\)

(12) 4' \((0,0,1/2), 0,0,1/2\)

(13) c' (0,0,1/2) x,0,z

(14) c' (0,0,1/2) 0,y,z

(15) m x,x,z

(16) m x,x,z
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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Symmetry of Special Projections

Along [0,0,1] \( \text{p4mm}' \)
- \( \mathbf{a}^* = \mathbf{a} \)
- \( \mathbf{b}^* = \mathbf{b} \)
- Origin at 0,0,z

Along [1,0,0] \( \text{p2''mm}' \)
- \( \mathbf{a}^* = -\mathbf{c}/2 \)
- \( \mathbf{b}^* = \mathbf{b} \)
- Origin at x,0,0

Along [1,1,0] \( \text{p2mm}' \)
- \( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \)
- \( \mathbf{b}^* = \mathbf{c} \)
- Origin at x,x,0
**Origin** at center \(( m'm'm )\) at \(4_2'/mc2'/m'\)

**Asymmetric unit** \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y\)

**Symmetry Operations**

1. \((1) \enspace 1\)
   \((1|0,0,0)\)

2. \((2) \enspace 2 \quad 0,0,z\)
   \((2_z|0,0,0)\)

3. \((3) \enspace 4^+ \times (0,0,1/2) \quad 0,0,z\)
   \((4_z|0,0,1/2)'\)

4. \((4) \enspace 4^- \times (0,0,1/2) \quad 0,0,z\)
   \((4_z^-|0,0,1/2)'\)

5. \((5) \enspace 2 \quad 0,y,1/4\)
   \((2_y|0,0,1/2)\)

6. \((6) \enspace 2 \quad x,0,1/4\)
   \((2_x|0,0,1/2)\)

7. \((7) \enspace 2' \quad x,x,0\)
   \((2_{xy}|0,0,0)'\)

8. \((8) \enspace 2' \quad x,x,0\)
   \((2_{xy}|0,0,0)'\)

9. \((9) \enspace \bar{1} \quad 0,0,0\)
   \((\bar{1}|0,0,0)\)

10. \((10) \enspace m \quad x,y,0\)
    \((m|0,0,0)\)

11. \((11) \enspace \bar{4}^- \times \quad 0,0,z; \quad 0,0,1/4\)
    \((\bar{4}_z|0,0,1/2)'\)

12. \((12) \enspace \bar{4}^- \times \quad 0,0,z; \quad 0,0,1/4\)
    \((\bar{4}_{z^-}|0,0,1/2)'\)

13. \((13) \enspace c \quad (0,0,1/2) \quad x,0,z\)
    \((m_y|0,0,1/2)\)

14. \((14) \enspace c \quad (0,0,1/2) \quad 0,y,z\)
    \((m_x|0,0,1/2)\)

15. \((15) \enspace m' \quad x,x,z\)
    \((m_x|0,0,0)'\)

16. \((16) \enspace m' \quad x,x,z\)
    \((m_x|0,0,0)'\)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<tr>
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<td>a</td>
<td>m..</td>
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<td></td>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>
**Symmetry of Special Projections**

Along \([0,0,1]\) \(\text{p}4\text{mm}'\)

- \(\mathbf{a}' = \mathbf{a}\)
- \(\mathbf{b}' = \mathbf{b}\)
- Origin at \(0,0,z\)

Along \([1,0,0]\) \(\text{p}_2\text{a}^* \ 2\text{m}'\text{m}'\)

- \(\mathbf{a}' = -\mathbf{c}/2\)
- \(\mathbf{b}' = \mathbf{b}\)
- Origin at \(x,0,1/4\)

Along \([1,1,0]\) \(\text{p}2'\text{mm}'\)

- \(\mathbf{a}' = -\mathbf{c}\)
- \(\mathbf{b}' = (-\mathbf{a} + \mathbf{b})/2\)
- Origin at \(x,x,0\)
Origin at center (mmm') at 42'/m'/c'2'/m

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

(1) 1
(1|0,0,0)

(5) 2 0,y,1/4
(2y|0,0,1/2)

(9) 1' 0,0,0
(1'|0,0,0')

(13) c' (0,0,1/2) x,0,z
(m|x|0,0,1/2')

(2) 2 0,0,z
(2z|0,0,0)

(6) 2 x,0,1/4
(2z|0,0,1/2)

(10) m' x,y,0
(m|0,0,0')

(14) c' (0,0,1/2) 0,y,z
(m|x|0,0,1/2')

(3) 4+ (0,0,1/2) 0,0,z
(4z|0,0,1/2')

(7) 2' x,x,0
(2x|0,0,0')

(11) 4+ 0,0,z; 0,0,1/4
(4z|0,0,1/2)

(8) 2' x,x,0
(2x|0,0,0')

(12) 4+ 0,0,z; 0,0,1/4
(4z|0,0,1/2)

(15) m x,x,z
(m|x|0,0,0)

(16) m x,x,z
(m|x|0,0,0)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y,x,z+1/2 [v,u,w]</td>
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<td>(7) y,x,z [v,u,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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<td>4 i m'.2m</td>
<td>x,x,0 [u,u,0]</td>
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<tr>
<td>2 c m'.mm</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] \( p4'm'm \)
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] \( p2m'm' \)
\( a^* = b \quad b^* = c/2 \)
Origin at x,0,1/4

Along [1,1,0] \( p2mm1' \)
\( a^* = (-a + b)/2 \quad b^* = c \)
Origin at x,x,0
Origin at center (m'm'm) at $4_{2}$/mc'2'/m'

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$; $x \leq y$

Symmetry Operations

1. $1$
   
   2. $2$  \( 0,0,z \)
      \( (2z,0,0) \)

5. $2'$  \( 0,y,1/4 \)
   \( (2\overline{y},0,1/2) \)

9. $1$  \( 0,0,0 \)
   \( (1,0,0) \)

13. $c'$  \( (0,0,1/2) \)
    \( (mz,0,1/2) \)

   14. $c'$  \( (0,0,1/2) \)
      \( (mz,0,1/2) \)

   15. $m'$  \( x,z \)
      \( (mz,0,0) \)

   16. $m'$  \( x,z \)
      \( (mz,0,0) \)

$P4_{2}$/mc'm'

$4_{2}$ /mc'2'/m'

$132.7.1116$

Tetragonal
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<td>x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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<tr>
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<td>x,y,0 [0,0,w]</td>
<td>y,x,1/2 [0,0,w]</td>
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<td>x,y,1/2 [0,0,w]</td>
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<td>8 m .2'</td>
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<td>x,1/2,1/4 [0,v,w]</td>
<td>1/2,x,3/4 [v,0,w]</td>
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<td>x,1/2,3/4 [0,v,w]</td>
<td>1/2,x,1/4 [v,0,w]</td>
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<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
<td>0,x,3/4 [v,0,w]</td>
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<td>x,0,3/4 [0,v,w]</td>
<td>x,0,3/4 [0,v,w]</td>
<td>0,x,1/4 [v,0,w]</td>
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<td>8 k .2'</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>0,1/2,z+1/2 [0,0,w]</td>
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<tr>
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<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 j m.2'</td>
<td>x,x,1/2 [0,0,w]</td>
<td>x,x,1/2 [0,0,w]</td>
<td>x,x,0 [0,0,w]</td>
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<tr>
<td>4 i m.2'</td>
<td>x,x,0 [0,0,w]</td>
<td>x,x,0 [0,0,w]</td>
<td>x,x,1/2 [0,0,w]</td>
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<tr>
<td>4 h 2.m'</td>
<td>1/2,1/2,z [0,0,w]</td>
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<tr>
<td>4 g 2.m'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
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<tr>
<td>4 f 2/m..</td>
<td>0,1/2,0 [0,0,w]</td>
<td>1/2,0,1/2 [0,0,w]</td>
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<td>1/2,0,3/4 [0,0,w]</td>
<td>0,1/2,3/4 [0,0,w]</td>
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<tr>
<td>2 d 42'2'</td>
<td>1/2,1/2,1/4 [0,0,w]</td>
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<td>1/2,1/2,3/4 [0,0,w]</td>
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<tr>
<td>2 c m.m'm'</td>
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<td>1/2,1/2,1/2 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 b 42'm'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
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<td>0,0,0 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] \( p'4mm' \)
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] \( p'2'mm' \)
\[ a^* = -c/2 \quad b^* = b \]
Origin at x,0,0

Along [1,1,0] \( p'2'mm' \)
\[ a^* = -c \quad b^* = (-a + b)/2 \]
Origin at x,x,0
**Origin** at center (m'm'm') at 4'/m'c2/m'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y \]

**Symmetry Operations**

1. \(1\)
   \((1|0,0,0)\)

2. \(2\)
   \(0,0,z\)
   \((2_z|0,0,0)\)

3. \(4^+\) (0,0,1/2)
   \(0,0,z\)
   \((4_z|0,0,1/2)'\)

4. \(4^-\) (0,0,1/2)
   \(0,0,z\)
   \((4_z^{-1}|0,0,1/2)'\)

5. \(2'\)
   \(0,0,1/4\)
   \((2_z|0,0,1/2)'\)

6. \(2'\)
   \(x,0,1/4\)
   \((2_x|0,0,1/2)'\)

7. \(2\)
   \(x,x,0\)
   \((2_xy|0,0,0)\)

8. \(2\)
   \(x,x,0\)
   \((2_{xy}|0,0,0)\)

9. \(\bar{1}\)
   \(0,0,0\)
   \((\bar{1}|0,0,0)'\)

10. \(m'\)
    \(x,y,0\)
    \((m_x|0,0,0)'\)

11. \(4^+\)
    \(0,0,z; 0,0,1/4\)
    \((4_z|0,0,1/2)\)

12. \(4^-\)
    \(0,0,z; 0,0,1/4\)
    \((4_z^{-1}|0,0,1/2)\)

13. \(c\)
    \((0,0,1/2)\)
    \(x,0,z\)
    \((m_x|0,0,1/2)\)

14. \(c\)
    \((0,0,1/2)\)
    \(0,y,z\)
    \((m_y|0,0,0)'\)

15. \(m'\)
    \(x,x,z\)
    \((m_{xy}|0,0,0)'\)

16. \(m'\)
    \(x,x,z\)
    \((m_{xy}|0,0,0)'\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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</table>

| 16 | p | 1 | (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] | (3) y,x,z+1/2 [v,u,w] | (4) y,x,z+1/2 [v,u,w] |
| (5) x,y,z+1/2 [u,v,w] | (6) x,y,z+1/2 [u,v,w] | (7) y,x,z [v,u,w] | (8) y,x,z [v,u,w] |
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| 8 | o | .m' | x,x,z [u,u,w] | x,x,z [u,u,w] | x,x,z+1/2 [u,u,w] | x,x,z+1/2 [u,u,w] |
| x,x,z+1/2 [u,u,w] | x,x,z+1/2 [u,u,w] |

| 8 | n | m'.. | x,y,0 [u,v,0] | x,y,0 [u,v,0] | y,x,1/2 [v,u,0] | y,x,1/2 [v,u,0] |
| x,y,1/2 [u,v,0] | x,y,1/2 [u,v,0] |

| 8 | m | .2' | x,1/2,1/4 [0,v,w] | x,1/2,1/4 [0,v,w] | 1/2,x,3/4 [v,0,w] | 1/2,x,3/4 [v,0,w] |
| x,1/2,3/4 [0,v,w] | x,1/2,3/4 [0,v,w] |

| 8 | l | .2' | x,0,1/4 [0,v,w] | x,0,1/4 [0,v,w] | 0,x,3/4 [v,0,w] | 0,x,3/4 [v,0,w] |
| x,0,3/4 [0,v,w] | x,0,3/4 [0,v,w] |

| 8 | k | 2.. | 0,1/2,z [0,0,w] | 0,1/2,z [0,0,w] | 1/2,0,z+1/2 [0,0,w] | 1/2,0,z+1/2 [0,0,w] |
| 0,1/2,z [0,0,w] | 0,1/2,z [0,0,w] |

| 4 | j | m'.2m' | x,x,1/2 [u,u,0] | x,x,1/2 [u,u,0] | x,x,0 [u,u,0] | x,x,0 [u,u,0] |
| x,x,0 [u,u,0] | x,x,0 [u,u,0] |

| 4 | i | m'.2m' | x,x,0 [u,u,0] | x,x,0 [u,u,0] | x,x,1/2 [u,u,0] | x,x,1/2 [u,u,0] |
| x,x,0 [u,u,0] | x,x,0 [u,u,0] |

| 4 | h | 2.m'm' | 1/2,1/2,z [0,0,w] | 1/2,1/2,z [0,0,w] | 1/2,1/2,z+1/2 [0,0,w] | 1/2,1/2,z+1/2 [0,0,w] |
| 1/2,1/2,z+1/2 [0,0,w] | 1/2,1/2,z+1/2 [0,0,w] |

| 4 | g | 2.m'm' | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z+1/2 [0,0,w] |
| 0,0,z+1/2 [0,0,w] | 0,0,z+1/2 [0,0,w] |

| 4 | f | 2/m'.. | 0,1/2,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |
| 1/2,0,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |

| 4 | e | 22'2'.. | 0,1/2,1/4 [0,0,w] | 0,1/2,1/4 [0,0,w] | 1/2,0,3/4 [0,0,w] | 1/2,0,3/4 [0,0,w] |
| 1/2,0,3/4 [0,0,w] | 1/2,0,3/4 [0,0,w] |

| 2 | d | 42'm' | 1/2,1/2,1/4 [0,0,w] | 1/2,1/2,1/4 [0,0,w] |
| 1/2,1/2,1/4 [0,0,w] | 1/2,1/2,1/4 [0,0,w] |

| 2 | c | m'.m'm' | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |

| 2 | b | 42'm' | 0,0,1/4 [0,0,w] | 0,0,1/4 [0,0,w] |
| 0,0,3/4 [0,0,w] | 0,0,3/4 [0,0,w] |

| 2 | a | m'.m'm' | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] |
| 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Translation</th>
<th>Rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p4'mm'</td>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p2m'm'</td>
<td>a* = -c/2</td>
<td>b* = b</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>p2m'm'</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center ($m'm'm'$) at $4/m'c'/2/m'$

Asymmetric unit

$$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y$$

Symmetry Operations

1. 1
2. $2 \cdot 0,0,z$
3. $4^+ \cdot (0,0,1/2)\cdot 0,0,z$
4. $4^- \cdot (0,0,1/2)\cdot 0,0,z$

5. $2 \cdot 0,y,1/4$
6. $2 \cdot x,0,1/4$
7. $2 \cdot x,x,0$
8. $2 \cdot x,x,0$

9. $\bar{1} \cdot 0,0,0$
10. $m' \cdot x,y,0$
11. $\bar{4}^+ \cdot 0,0,z; 0,0,1/4$
12. $\bar{4}^- \cdot 0,0,z; 0,0,1/4$

13. $c' \cdot (0,0,1/2)\cdot x,0,z$
14. $c' \cdot (0,0,1/2)\cdot 0,y,z$
15. $m' \cdot x,x,z$
16. $m' \cdot x,x,z$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 p 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z+1/2 [v,u,w] (4) x,y,z+1/2 [v,u,w] (5) x,y,z+1/2 [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) y,x,z [v,u,w] (8) y,x,z [v,u,w] (9) x,y,z [u,v,w] (10) x,y,z [u,v,w] (11) x,y,z [u,v,w] (12) x,y,z [u,v,w] (13) x,y,z [u,v,w] (14) x,y,z [u,v,w] (15) x,y,z [v,u,w] (16) x,y,z [v,u,w]</td>
</tr>
<tr>
<td>8 o .m'</td>
<td>x,x,z [u,u,w] x,x,z+1/2 [u,u,w] x,x,z+1/2 [u,u,w] x,x,z+1/2 [u,u,w] x,x,z+1/2 [u,u,w] x,x,z+1/2 [u,u,w] x,x,z+1/2 [u,u,w] x,x,z+1/2 [u,u,w]</td>
</tr>
<tr>
<td>8 n m'..</td>
<td>x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0] x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>8 m .2.</td>
<td>x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0]</td>
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<tr>
<td>8 l .2.</td>
<td>x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>8 k 2..</td>
<td>0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 j m'.2m'</td>
<td>x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td>4 i m'.2m'</td>
<td>x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>4 h 2.m'm'</td>
<td>1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 g 2.m'm'</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 f 2/m'..</td>
<td>0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4 e 222.</td>
<td>0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2 d 422m'</td>
<td>1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0] 1/2,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2 c m'.m'm'</td>
<td>1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 b 422m'</td>
<td>0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0]</td>
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<tr>
<td>2 a m'.m'm'</td>
<td>0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0] 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1]  p4m'm'
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0]  p 2m'm'
\[ a^* = b \quad b^* = c/2 \]
Origin at x,0,0

Along [1,1,0]  p2m'm'
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,0
Origin at center (mmm) at $4_2/\text{mc2/m}$

Asymmetric unit

$$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y$$

Symmetry Operations

For $(0,0,0)$ set

1. $1$
   
2. $2 \cdot 0,0,z$
   
3. $4^+ (0,0,1/2) \cdot 0,0,z$
   
4. $4^- (0,0,1/2) \cdot 0,0,z$
   
5. $2 \cdot 0,y,1/4$
   
6. $2 \cdot x,0,1/4$
   
7. $2 \cdot x,x,0$

8. $2 \cdot x,0,0$

9. $1 \cdot 0,0,0$

10. $m \cdot x,y,0$

11. $4^+ \cdot 0,0,z; 0,0,1/4$

12. $4^- \cdot 0,0,z; 0,0,1/4$

13. $c \cdot (0,0,1/2) \cdot x,0,z$

14. $c \cdot (0,0,1/2) \cdot 0,y,z$

15. $m \cdot x,x,z$

16. $m \cdot x,x,z$
Continued

For \(1,0,0\)' + set

(1) \(t' (1,0,0)\)
(2) \(2' 1/2,0,z\)
(3) \(4^+ (0,0,1/2) 1/2,1/2,z\)
(4) \(4^- (0,0,1/2) 1/2,-1/2,z\)

(5) \(2' 1/2,0,1/4\)
(6) \(2' (1,0,0) 0,1/4\)
(7) \(2' (1/2,1/2,0) x+1/2,x,0\)
(8) \(2' (1/2,-1/2,0) x+1/2,x,0\)

(9) \(T' 1/2,0.0\)
(10) \(a' (1,0,0) x,y,0\)
(11) \(4^+ (1/2,-1/2,0) x+1/2,x,0\)
(12) \(4^- (1/2,1/2,0) x+1/2,x,0\)

(13) \(n' (1,0,1/2) x,0,z\)
(14) \(c' (0,0,1/2) 1/2,y,z\)
(15) \(g' (1/2,-1/2,0) x+1/2,x\)
(16) \(g' (1/2,1/2,0) x+1/2,x\)

Generators selected (1); \(t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 p 1</td>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>u,v,w</td>
<td></td>
</tr>
<tr>
<td>(2) x,y,z</td>
<td>u,v,w</td>
<td></td>
</tr>
<tr>
<td>(3) y,x,z+1/2</td>
<td>v,u,w</td>
<td></td>
</tr>
<tr>
<td>(4) y,x,z+1/2</td>
<td>v,u,w</td>
<td></td>
</tr>
<tr>
<td>(5) x,y,z+1/2</td>
<td>u,v,w</td>
<td></td>
</tr>
<tr>
<td>(6) x,y,z+1/2</td>
<td>u,v,w</td>
<td></td>
</tr>
<tr>
<td>(7) y,x,z</td>
<td>v,u,w</td>
<td></td>
</tr>
<tr>
<td>(8) y,x,z</td>
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<tr>
<td>(9) x,y,z</td>
<td>u,v,w</td>
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<tr>
<td>(10) x,y,z</td>
<td>u,v,w</td>
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<tr>
<td>(11) y,x,z+1/2</td>
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<td>(12) y,x,z+1/2</td>
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<td>(13) x,y,z+1/2</td>
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<tr>
<td>(14) x,y,z+1/2</td>
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<td>(15) y,x,z</td>
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<tr>
<td>(16) y,x,z</td>
<td>v,u,w</td>
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</tbody>
</table>

16 o .m x,x,z [u,u,0] x,x,z [u,u,0] x,x,z+1/2 [u,u,0] x,x,z x,x,z [u,u,0] x,x,z+1/2 [u,u,0]

16 n m.. x,y,0 [0,0,w] x,y,0 [0,0,w] y,x,1/2 [0,0,w] y,x,1/2 [0,0,w] y,x,0 [0,0,w] y,x,0 [0,0,w]

16 m .2' x,1/2,1/4 [0,v,w] x,1/2,1/4 [0,v,w] 1/2,x,3/4 [v,0,w] 1/2,x,3/4 [v,0,w] 1/2,x,1/4 [v,0,w] 1/2,x,1/4 [v,0,w]

16 l .2 x,0,1/4 [u,0,0] x,0,1/4 [u,0,0] 0,x,3/4 [0,u,0] 0,x,3/4 [0,u,0] 0,x,1/4 [0,u,0] 0,x,1/4 [0,u,0]

16 k 2'.. 0,1/2,z [u,v,0] 0,1/2,z [u,v,0] 1/2,0,z+1/2 [v,u,0] 1/2,0,z+1/2 [v,u,0] 1/2,0,z [v,u,0] 1/2,0,z [v,u,0]

8 j m.2m x,x,1/2 [0,0,0] x,x,1/2 [0,0,0] x,x,0 [0,0,0] x,x,0 [0,0,0] x,x,0 [0,0,0] x,x,0 [0,0,0]

8 i m.2m x,x,0 [0,0,0] x,x,0 [0,0,0] x,x,1/2 [0,0,0] x,x,1/2 [0,0,0] x,x,1/2 [0,0,0] x,x,1/2 [0,0,0]

8 h 2.mm 1/2,1/2,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 1/2,1/2,z [0,0,0] 1/2,1/2,z [0,0,0]

16 1/2,1/2,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 1/2,1/2,z [0,0,0] 1/2,1/2,z [0,0,0]
Symmetry of Special Projections

Along [0,0,1] p4mm1'
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p2mm1'
\( a^* = b \quad b^* = c/2 \)
Origin at x,0,0

Along [1,1,0] p2mm1'
\( a^* = (-a + b)/2 \quad b^* = c \)
Origin at x,x,0
Origin at center (mmm') at $4_2/m'c'2/m$

Asymmetric unit

$$\begin{align*}
0 & \leq x \leq 1/2; \\
0 & \leq y \leq 1/2; \\
0 & \leq z \leq 1/2; \\
x & < y
\end{align*}$$

Symmetry Operations

For (0,0,0) + set

1. $\begin{pmatrix} 1 \end{pmatrix}$
2. $\begin{pmatrix} 2 \end{pmatrix}$ $0,0,z$
   $(2z|0,0,0)$
3. $\begin{pmatrix} 4^+ \end{pmatrix}$ $(0,0,1/2)0,0,z$
   $(4_2|0,0,1/2)$
4. $\begin{pmatrix} 4^- \end{pmatrix}$ $(0,0,1/2)0,0,z$
   $(4_2^{-1}|0,0,1/2)$
5. $\begin{pmatrix} 2' \end{pmatrix}$ $0,y,1/4$
   $(2_2|0,0,1/2)'$
6. $\begin{pmatrix} 2' \end{pmatrix}$ $x,0,1/4$
   $(2_z|0,0,1/2)'$
7. $\begin{pmatrix} 2' \end{pmatrix}$ $x,x,0$
   $(2_{xy}|0,0,0)'$
8. $\begin{pmatrix} 2' \end{pmatrix}$ $x,x,0$
   $(2_{xy}|0,0,0)'$
9. $\begin{pmatrix} 1' \end{pmatrix}$ $0,0,0$
   $(1|0,0,0)'$
10. $\begin{pmatrix} m' \end{pmatrix}$ $x,y,0$
    $(m_z|0,0,0)'$
11. $\begin{pmatrix} 4^{+}\overline{1} \end{pmatrix}$ $0,0,z; 0,0,1/4$
    $(4_z^{-1}|0,0,1/2)'$
12. $\begin{pmatrix} 4^{-}\overline{1} \end{pmatrix}$ $0,0,z; 0,0,1/4$
    $(4_z^{-1}|0,0,1/2)'$
13. $\begin{pmatrix} c \end{pmatrix}$ $(0,0,1/2) x,0,z$
    $(m_1|0,0,1/2)$
14. $\begin{pmatrix} c \end{pmatrix}$ $(0,0,1/2) 0,y,z$
    $(m_z|0,0,1/2)$
15. $\begin{pmatrix} m \end{pmatrix}$ $x,x,z$
    $(m_{xy}|0,0,0)$
16. $\begin{pmatrix} m \end{pmatrix}$ $x,x,z$
    $(m_{xy}|0,0,0)$
Continued

For (1,0,0)'+ set

(1) t' (1,0,0)   (2) 2' 1/2,0,z (3) 4' (0,0,1/2) 1/2,1/2,z (4) 4' (0,0,1/2) 1/2,-1/2,z
   (1 1,0,0)'   (2 1/2,0,0)'   (3 1/2,0,1/2)'   (4 1/2,0,1/2)'  

(5) 2 1/2,y,1/4   (6) 2 (1,0,0) x,0,1/4 (7) 2 (1/2,1/2,0) x+1/2,x,0 (8) 2 (1/2,-1/2,0)
   (2 1/2,1/2)'   (2 1/2,1/2)'  

(9) T 1/2,0,0    (10) a (1,0,0) x,y,0 (11) 4' 1/2,-1/2,z; 1/2,-1/2,1/4
   (T 1/0,0)     (m 1/0,0)     (4 1/2,1/2,1/4)  

(13) n' (1,0,1/2) x,0,z (14) c' (0,0,1/2) 1/2,y,z (15) g' (1/2,-1/2,0) x+1/2,x,z
   (m 1,0,1/2)'  (m 1,0,1/2)'  (m 1/2,1/2,1/4)  

Generators selected
(1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 p 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(1,0,0)'+</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
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<td></td>
<td>(7) y,x,z [v,u,w]</td>
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<td></td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(11) y,x,z+1/2 [v,u,w]</td>
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<td>(15) y,x,z [v,u,w]</td>
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<td></td>
<td>(16) y,0 [u,v,w]</td>
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<tr>
<td></td>
<td>(17) x,y,0 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(18) y,x,0 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(19) y,x,0 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(20) x,0,1/4 [0,v,w]</td>
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<tr>
<td></td>
<td>(21) x,0,1/4 [0,v,w]</td>
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<td></td>
<td>(22) x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>(23) x,0,1/4 [0,v,w]</td>
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<td></td>
<td>(24) x,0,1/4 [0,v,w]</td>
</tr>
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<td></td>
<td>(25) x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>(26) x,0,1/4 [0,v,w]</td>
</tr>
</tbody>
</table>

16 o ..m x,x,z [u,u,0] x,x,z [u,u,0] x,x,z [u,u,0] x,x,z [u,u,0]

16 n m'.. x,y,0 [u,v,0] x,y,0 [u,v,0] y,x,1/2 [v,u,0] y,x,1/2 [v,u,0]

16 m .2. x,1/2,1/4 [u,0,0] x,1/2,1/4 [u,0,0] x,u,3/4 [0,u,0] x,u,3/4 [0,u,0]

16 l .2'. x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] 0,x,3/4 [v,0,w] 0,x,3/4 [v,0,w]

16 k 2'. 0,1/2,z [u,v,0] 0,1/2,z [u,v,0] 0,1/2,z [u,v,0] 0,1/2,z [u,v,0]

8 j m'.2'm x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0] x,x,1/2 [u,u,0]
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>8</th>
<th>h</th>
<th>2.mm</th>
<th>1/2,1/2,z [0,0,0]</th>
<th>1/2,1/2,z+1/2 [0,0,0]</th>
<th>1/2,1/2,\bar{z}+1/2 [0,0,0]</th>
<th>1/2,1/2,\bar{z} [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>g</td>
<td>2.mm</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
<td>0,0,\bar{z}+1/2 [0,0,0]</td>
<td>0,0,\bar{z} [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>2'/m'..</td>
<td>0,1/2,0 [u,v,0]</td>
<td>1/2,0,1/2 [v,u,0]</td>
<td>0,1/2,1/2 [u,v,0]</td>
<td>1/2,0,0, [v,u,0]</td>
</tr>
<tr>
<td>8</td>
<td>e</td>
<td>2'2'.</td>
<td>0,1/2,1/4 [u,0,0]</td>
<td>1/2,0,3/4 [0,u,0]</td>
<td>0,1/2,3/4 [u,0,0]</td>
<td>1/2,0,1/4 [0,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>\bar{4}2m</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>m'.mm</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,2 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>\bar{4}'2'm</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>m'.mm</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p\text{p\prime}, 4mm

\begin{align*}
\mathbf{a}^* &= \mathbf{a} & \mathbf{b}^* &= \mathbf{b} \\
\text{Origin at } 0,0,z
\end{align*}

Along [1,0,0] p2mm1'

\begin{align*}
\mathbf{a}^* &= \mathbf{b} & \mathbf{b}^* &= \mathbf{c} \\
\text{Origin at } x,0,0
\end{align*}

Along [1,1,0] p2mm1'

\begin{align*}
\mathbf{a}^* &= (-\mathbf{a} + \mathbf{b})/2 & \mathbf{b}^* &= \mathbf{c} \\
\text{Origin at } x,x,0
\end{align*}
Pₚ 4₂'/mcm'  
132.12.1121  

4/mmm1'  
Pₚ 4₂'/m2/c2'/m'  

Tetragonal

Origin at center (m'm'm) at 4₂'/mc2'/m'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x < y

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)  
(2) 2 0,0,z  
(2z|0,0,0)  
(3) 4⁺ 0,0,1/2 0,0,z  
(4z|0,0,1/2)  
(4) 4⁻ 0,0,1/2 0,0,z  
(4z⁻|0,0,1/2)  

(5) 2 0,y,1/4  
(2|0,0,1/2)  
(6) 2 x,0,1/4  
(2z|0,0,1/2)  
(7) 2⁺ x,x,0  
(2xy|0,0,0)  
(8) 2⁻ x,x,0  
(2xy|0,0,0)  

(9) 1 0,0,0  
(1|0,0,0)  
(10) m x,y,0  
(mz|0,0,0)  
(11) 4⁺ 0,0,z; 0,0,1/4  
(4z|0,0,1/2)  
(12) 4⁻ 0,0,z; 0,0,1/4  
(4z⁻|0,0,1/2)  

(13) c (0,0,1/2) x,0,z  
(m|0,0,1/2)  
(14) c (0,0,1/2) 0,y,z  
(m|0,0,1/2)  
(15) m' x,x,z  
(mxy|0,0,0)  
(16) m' x,x,z  
(mxy|0,0,0)
Continued

For \((1,0,0)\) + set

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>((1)) (t'(1,0,0)) ((1)) ((1,0,0))' ((1)) ((1,0,0))'</td>
</tr>
<tr>
<td>(32)</td>
<td>(p)</td>
</tr>
<tr>
<td>(5)</td>
<td>(2') (1/2, y, 1/4) ((5)) ((2,1,0,1/2))' (2) ((2,1,0,1/2))'</td>
</tr>
<tr>
<td>(9)</td>
<td>(\bar{T}) (1/2,0,0) ((9)) ((m,1,0,0))' ((9)) ((m,1,0,0))'</td>
</tr>
<tr>
<td>(13)</td>
<td>(n') ((1,0,1/2)) (x,0, z) ((13)) ((m,1,0,1/2))' ((13)) ((m,1,0,1/2))'</td>
</tr>
</tbody>
</table>

Positions selected \((1); t'(1,0,0); t'(0,1,0); t(0,0,1); (2); (3); (5); (9).\)

Multiplicity,
Wyckoff letter,
Site Symmetry.
| 8  | g   | 2\text{.m'}m' | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z [0,0,w] |
| 8  | f   | 2'/m.. | 0,1/2,0 [0,0,0] | 1/2,0,1/2 [0,0,0] | 0,1/2,1/2 [0,0,0] | 1/2,0,0, [0,0,0] |
| 8  | e   | 2'2'2'. | 0,1/2,1/4 [0,v,0] | 1/2,0,3/4 [v,0,0] | 0,1/2,3/4 [0,v,0] | 1/2,0,1/4 [0,v,0] |
| 4  | d   | 4'2'm' | 1/2,1/2,1/4 [0,0,w] | 1/2,1/2,3/4 [0,0,w] | | |
| 4  | c   | m.mm  | 1/2,1/2,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] | | |
| 4  | b   | 4'2m' | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] | | |
| 4  | a   | m.m'm' | 0,0,0 [0,0,w] | 0,0,1/2 [0,0,w] | | |

**Symmetry of Special Projections**

- Along [0,0,1] p4mm1'
  - \(a^* = a\) \(b^* = b\)
  - Origin at 0,0,z

- Along [1,0,0] p2mm1'
  - \(a^* = b\) \(b^* = c/2\)
  - Origin at x,0,0

- Along [1,1,0] p_{2\alpha} 2mm
  - \(a^* = -c\) \(b^* = (a + b)/2\)
  - Origin at x-1/4,x+1/4,0
Origin at center (m'm'm') at 4/m'/c2/m'

Asymmetric unit

\(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\)

(1) \(1\) 
(1) \((0,0,0)\)

2. \(2\)

(2) \(2\) 0,0,0  
\(2_z\) 0,0,0

3. \(4'\)

(3) \(4'\) (0,0,1/2) 0,0,0  
\(4_z\) (0,0,1/2)' 

4. \(4'\)

(4) \(4'\) (0,0,1/2) 0,0,0  
\(4_z\) (0,0,1/2)'

5. \(2'\)

(5) \(2'\) 0,y,1/4  
\(2_y\) 0,0,1/2)

6. \(2'\)

(6) \(2'\) x,0,1/4  
\(2_x\) 0,0,1/2)

7. \(2\)

(7) \(2\) x,x,0  
\(2_x\) 0,0,0

8. \(2\)

(8) \(2\) x,x,0  
\(2_y\) 0,0,0

9. \(\bar{1}\)

(9) \(\bar{1}\) 0,0,0  
\(\bar{1}_y\) 0,0,0)

10. \(m'\)

(10) \(m'\) x,y,0 
\(m_x\) 0,0,0)'

11. \(\bar{4}\)

(11) \(\bar{4}\) 0,0,0; 0,0,1/4  
\(\bar{4}_y\) 0,0,1/2)

12. \(\bar{4}\)

(12) \(\bar{4}\) 0,0,0; 0,0,1/4  
\(\bar{4}_y\) 0,0,1/2)

13. \(c\)

(13) \(c\) (0,0,1/2) x,0,0  
\(c_x\) 0,0,1/2)

14. \(c\)

(14) \(c\) (0,0,1/2) 0,y,0  
\(c_x\) 0,0,1/2)

15. \(m'\)

(15) \(m'\) x,y,z  
\(m_y\) 0,0,0)'

16. \(m'\)

(16) \(m'\) x,x,z  
\(m_{xy}\) 0,0,0)'

132.13.1122 - 1 - 2332
Continued

For \((1,0,0)\)' + set

(1) \(t'(1,0,0)\)
(2) \(2' \ 1/2,0,z\)
(3) \(4' \ (0,0,1/2) \ 1/2,1/2,z\)
(4) \(4' \ (0,0,1/2) \ 1/2,-1/2,z\)

(5) 2 1/2,y,1/4
(2') 1,0,1/2

(6) 2' (1,0,0) x,0,1/4
(2') 1,0,1/2

(7) 2' (1/2,1/2,0) x+1,2,x,0
(2') 1,0,1/2

(8) 2' (1/2,-1/2,0) x+1,2,x,0
(2') 1,0,1/2

(9) \(T \ 1/2,0,0\)

(10) a (1,0,0) x,y,0
(2') 1,0,1/2

(11) \(4' \ (1,0,1/2) \ 1/2,1/2,z\)
(4') 1,0,1/2

(12) \(4' \ (1,0,0) \ 1/2,1/2,z\)
(4') 1,0,1/2

(13) \(n' (1,0,1/2) \ x,0,z\)

(14) \(c' (0,0,1/2) \ 1/2,y,z\)

(15) \(g (1/2,-1/2,0) \ x+1/2,x,0\)

(16) \(g (1/2,1/2,0) \ x+1/2,x,0\)

Generators selected

\((1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (9).\)

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.
Coordinates

\((0,0,0)\) + \((1,0,0)\)'

16 o 
\(x,y,z [u,v,w]\) 
\(x,y,z [u,v,w]\)
\(x,y,z+1/2 [u,v,w]\)
\(x,y,z+1/2 [u,v,w]\)

16 n 
\(x,y,0 [u,v,0]\) 
\(x,y,0 [u,v,0]\)
\(y,x,1/2 [v,u,0]\)
\(y,x,1/2 [v,u,0]\)

16 m 
\(x,1/2,1/4 [u,0,0]\)
\(x,1/2,1/4 [u,0,0]\)
\(1/2,x,3/4 [0,u,0]\)
\(1/2,x,3/4 [0,u,0]\)

16 l 
\(x,0,1/4 [0,v,w]\)
\(x,0,1/4 [0,v,w]\)
\(0,x,3/4 [v,0,w]\)
\(0,x,3/4 [v,0,w]\)

16 k 
\(0,1/2,z [u,v,0]\)
\(0,1/2,z [u,v,0]\)
\(0,1/2,z+1/2 [v,u,0]\)
\(0,1/2,z+1/2 [v,u,0]\)

8 j 
\(x,x,1/2 [u,u,0]\)
\(x,x,0 [u,u,0]\)
\(x,x,0 [u,u,0]\)
\(x,x,1/2 [u,u,0]\)

8 i 
\(x,x,0 [u,u,0]\)
\(x,x,0 [u,u,0]\)
\(x,x,0 [u,u,0]\)
\(x,x,1/2 [u,u,0]\)

8 h 2mm 
\(1/2,1/2,z [0,0,0]\)
\(1/2,1/2,z+1/2 [0,0,0]\)
\(1/2,1/2,z+1/2 [0,0,0]\)
\(1/2,1/2,z+1/2 [0,0,0]\)
Continued

| 8 | g   | 2.m'm' | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z [0,0,w] |
| 8 | f   | 2'/m' | 0,1/2,0 [u,v,0] | 1/2,0,1/2 [v,u,0] | 0,1/2,1/2 [u,v,0] |
| 8 | e   | 2'22' | 0,1/2,1/4 [u,0,0] | 1/2,0,3/4 [u,0,0] | 0,1/2,3/4 [u,0,0] |
| 4 | d   | 42'm' | 1/2,1/2,1/4 [0,0,0] | 1/2,1/2,3/4 [0,0,0] | 1/2,0,1/4 [0,0,0] |
| 4 | c   | m'.m'm' | 1/2,1/2,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] | 1/2,0,0, [v,u,0] |
| 4 | b   | 42'm' | 0,0,1/4 [0,0,w] | 0,0,3/4 [0,0,w] | 0,0,1/2 [0,0,w] |
| 4 | a   | m'.m'm' | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,2 [0,0,0] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p2 4m'm'</th>
<th>Along [1,0,0] p2mm1'</th>
<th>Along [1,1,0] p2a' 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{a^<em>} = \mathbf{a} ) ( \mathbf{b^</em>} = \mathbf{b} )</td>
<td>( \mathbf{a^<em>} = \mathbf{b} ) ( \mathbf{b^</em>} = \mathbf{c}/2 )</td>
<td>( \mathbf{a^<em>} = (-\mathbf{a} + \mathbf{b})/2 ) ( \mathbf{b^</em>} = \mathbf{c} )</td>
</tr>
<tr>
<td>Origin at 1/2,1/2,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin at \( \bar{4}12_{1}/c \), at \(-1/4,1/4,-1/4\) from \( \bar{1} \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1 | 0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2_{z} | 0,0,0) \\
(3) & \quad 4^{+} \quad (0,0,1/2) \quad 0,1/2,z \\
& \quad (4_{z} | 1/2,1/2,1/2) \\
(4) & \quad 4^{-} \quad (0,0,1/2) \quad 1/2,0,z \\
& \quad (4_{z}^{-} | 1/2,1/2,1/2) \\
(5) & \quad 2 \quad 0,y,1/4 \\
& \quad (2_{y} | 0,0,1/2) \\
(6) & \quad 2 \quad x,0,1/4 \\
& \quad (2_{x} | 0,0,1/2) \\
(7) & \quad 2 \quad (1/2,1/2,0) \quad x,x,0 \\
& \quad (2_{x,y} | 1/2,1/2,0) \\
(8) & \quad 2 \quad x,x+1/2,0 \\
& \quad (2_{x,y} | 1/2,1/2,0) \\
(9) & \quad \bar{1} \quad 1/4,1/4,1/4 \\
& \quad (1 \ | 1/2,1/2,1/2) \\
(10) & \quad n \quad (1/2,1/2,0) \quad x,y,1/4 \\
& \quad (m_{x,y} | 1/2,1/2,1/2) \\
(11) & \quad \bar{4}^{+} \quad 0,0,z; \quad 0,0,0 \\
& \quad (4_{z} | 0,0,0) \\
(12) & \quad \bar{4}^{-} \quad 0,0,z; \quad 0,0,0 \\
& \quad (4_{z}^{-} | 0,0,0) \\
(13) & \quad a \quad (1/2,0,0) \quad x,1/4,z \\
& \quad (m_{x} | 1/2,1/2,0) \\
(14) & \quad b \quad (0,1/2,0) \quad 1/4,y,z \\
& \quad (m_{y} | 1/2,1/2,0) \\
(15) & \quad c \quad (0,0,1/2) \quad x,x,z \\
& \quad (m_{x,y} | 0,0,1/2) \\
(16) & \quad c \quad (0,0,1/2) \quad x,x,z \\
& \quad (m_{x,y} | 0,0,1/2)
\end{align*}
\]
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Positions</th>
</tr>
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<tbody>
<tr>
<td>16 k 1</td>
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<td>(1) x,y,z [u,v,w] (2) x̅,y, z [u̅,v̅,w]</td>
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<tr>
<td></td>
<td></td>
<td>(3) y̅+1/2,x+1/2,z+1/2 [v̅,u,w] (4) y+1/2,x̅+1/2,z+1/2 [v̅,u̅,w]</td>
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<td></td>
<td>(5) x̅,y̅,z+1/2 [u̅,v,w] (6) x̅,y,z+1/2 [u̅,v̅,w]</td>
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<tr>
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<td></td>
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<tr>
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<td></td>
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<td></td>
<td>(15) y̅, x̅,z+1/2 [v̅,u,w] (16) y̅, x̅,z+1/2 [v̅,u̅,w]</td>
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<td>x̅+1/2,0 [u,u̅,0]</td>
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<td></td>
<td>x̅+1/2,1/2 [u,u̅,0]</td>
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<td>x̅+1/2,1/2,1/4 [u,u̅,0]</td>
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<td>x̅+1/2,1/2,1/4 [u,u̅,0]</td>
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<td>0,0,z [0,0,w]</td>
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<td>0,1/2,z [0,0,w]</td>
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<td>1/4,1/4,1/4 [u̅,v̅,w]</td>
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<td>0,0,0 [0,0,w]</td>
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<td>0,1/2,0 [0,0,0]</td>
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<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>4 b 222</td>
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<tr>
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<td>0,1/2,1/4 [0,0,0]</td>
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**Continued**
## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Formulae</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>pₐₜ, 4m'm'</td>
<td>$a^* = (a - b)/2$</td>
<td>1/2,0,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = (a + b)/2$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>Origin at 1/2,0,0</strong></td>
<td></td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p₂ₐₜ, 2m'm'</td>
<td>$a^* = b/2$</td>
<td>x,0,1/4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = c$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>Origin at x,0,1/4</strong></td>
<td></td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>p₂ₐₜ, 2m'm'</td>
<td>$a^* = -c/2$</td>
<td>x,x,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = (-a + b)/2$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>Origin at x,x,0</strong></td>
<td></td>
</tr>
</tbody>
</table>
Origin at $\overline{4} 12_i / c 1'$, at -1/4,1/4,-1/4 from $\overline{1}$ 1'

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

For 1 + set

1. $1$
   
   (1) $1$
   
   (2) $2 \cdot 0,0,z$
   
   (3) $4^+ (0,0,1/2) 0,1/2,z$
   
   (4) $4^- (0,0,1/2) 1/2,0,z$

2. $0,0,1/2$
   
   (2z) $0,0,0$

3. $0,1/2,0$
   
   (2x) $0,0,1/2$

4. $1/2,1/2,0$
   
   (4z) $1/2,1/2,1/2$

5. $0,0,1/2$
   
   (4z) $0,0,0$

6. $0,0,1/2$
   
   (4z) $0,0,0$

7. $1/2,1/2,0$
   
   (2x) $1/2,1/2,0$

8. $x,x+1/2,0$
   
   (2x) $1/2,1/2,0$

9. $1/4,1/4,1/4$
   
   (1) $1/2,1/2,1/2$

10. $1/4,1/4,1/4$
   
   (mz) $1/2,1/2,1/2$

11. $0,0,0$
   
   (mz) $0,0,0$

12. $0,0,0$
   
   (mz) $0,0,0$

13. $1/2,0,0$
   
   (mz) $1/2,1/2,0$

14. $1/4,1/4,1/4$
   
   (mz) $1/2,1/2,1/2$

15. $0,0,1/2$
   
   (mz) $0,0,1/2$

16. $0,0,1/2$
   
   (mz) $0,0,1/2$
Continued 133.2.1124 P4₁ /nbc₁'

For 1' + set

<table>
<thead>
<tr>
<th>(1) 1'</th>
<th>(2) 2'</th>
<th>(3) 4⁺'</th>
<th>(4) 4⁻'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1 0 0 0)⁺'</td>
<td>0 0 z</td>
<td>(0 0 1/2) 0 1/2 z</td>
<td>(0 0 1/2) 1/2 0 z</td>
</tr>
<tr>
<td>(2 0 0 0)⁺'</td>
<td>1/2 1/2 1/2 z⁺'</td>
<td>1/2 1/2 1/2 z⁺'</td>
<td></td>
</tr>
</tbody>
</table>

| (5) 2' 0, y, 1/4 | (6) 2' x, 0, 1/4 | (7) 2' (1/2, 1/2, 0) x, x, 0 | (8) 2' x, x + 1/2, 0 |
| (2 0 0 0 1/2)⁺' | (2 0 0 0 1/2)⁺' | (2 0 0 1/2 1/2, 1/2)⁺' | (2 0 0 1/2 1/2, 1/2)⁺' |

| (9) T⁺ 1/4, 1/4, 1/4 | (10) n⁺ (1/2, 1/2, 2) x, y, 1/4 | (11) 4⁺ x, 0, z; 0, 0, 0 | (12) 4⁻ x, 0, z; 0, 0, 0 |
| (1/2 1/2 1/2 1/2)⁺' | (m 1/2 1/2 1/2 1/2)⁺' | (4 0 0 0)⁺' | (4 z⁻ 0 0 0)⁺' |

| (13) a⁺ (1/2, 0, 0) x, 1/4, z | (14) b⁺ (0, 1/2, 0) 1/4, y, z | (15) c⁺ (0, 0, 1/2) x, x, z | (16) c⁻ (0, 0, 1/2) x, x, z |
| (m 1/2 1/2 1/2 1/2)⁺' | (m 1/2 1/2 1/2 1/2)⁺' | (m 0 0 1/2 1/2)⁺' | (m 0 0 1/2 1/2)⁺' |

Generators selected (1); t(1, 0, 0); t(0, 1, 0); t(0, 0, 1); (2); (3); (5); (9); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<th>1' +</th>
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<table>
<thead>
<tr>
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<th>11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x, y, z [0, 0, 0]</td>
<td>(2) x, y, z [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>(3) y + 1/2, x + 1/2, z + 1/2 [0, 0, 0]</td>
<td>(4) y + 1/2, x + 1/2, z + 1/2 [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>(5) x, y, z + 1/2 [0, 0, 0]</td>
<td>(6) x, y, z + 1/2 [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>(7) y + 1/2, x + 1/2, z [0, 0, 0]</td>
<td>(8) y + 1/2, x + 1/2, z [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>(9) x + 1/2, y + 1/2, z + 1/2 [0, 0, 0]</td>
<td>(10) x + 1/2, y + 1/2, z + 1/2 [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td>(11) y, x, z [0, 0, 0]</td>
<td>(12) y, x, z [0, 0, 0]</td>
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</tr>
<tr>
<td>(13) x + 1/2, y + 1/2, z [0, 0, 0]</td>
<td>(14) x + 1/2, y + 1/2, z [0, 0, 0]</td>
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</tr>
<tr>
<td>(15) y, x, z + 1/2 [0, 0, 0]</td>
<td>(16) y, x, z + 1/2 [0, 0, 0]</td>
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</table>

<table>
<thead>
<tr>
<th>8</th>
<th>j</th>
<th>.21'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x, x + 1/2, 0 [0, 0, 0])</td>
<td>x, x + 1/2, [0, 0, 0]</td>
<td>x, x + 1/2, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>x + 1/2, x, 1/2 [0, 0, 0]</td>
<td>x + 1/2, x, 1/2 [0, 0, 0]</td>
<td>x + 1/2, x, 0 [0, 0, 0]</td>
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<table>
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<tr>
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<th>i</th>
<th>.21'</th>
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<tbody>
<tr>
<td>x, 3/4 [0, 0, 0]</td>
<td>x, 3/4 [0, 0, 0]</td>
<td>1/2, x + 1/2, 1/4 [0, 0, 0]</td>
</tr>
<tr>
<td>x + 1/2, 1/2, 3/4 [0, 0, 0]</td>
<td>x + 1/2, 1/2, 3/4 [0, 0, 0]</td>
<td>0, x, 1/4 [0, 0, 0]</td>
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<tr>
<td>x, 1/4 [0, 0, 0]</td>
<td>x, 1/4 [0, 0, 0]</td>
<td>1/2, x + 1/2, 3/4 [0, 0, 0]</td>
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<tr>
<td>x + 1/2, 1/2, 1/4 [0, 0, 0]</td>
<td>x + 1/2, 1/2, 1/4 [0, 0, 0]</td>
<td>0, x, 3/4 [0, 0, 0]</td>
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<tbody>
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<td>0, 0, z [0, 0, 0]</td>
<td>0, 0, z [0, 0, 0]</td>
<td>0, z + 1/2 [0, 0, 0]</td>
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<tr>
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# Symmetry of Special Projections

<table>
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<tr>
<th>Operation</th>
<th>Axes</th>
<th>Special Projections</th>
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<tbody>
<tr>
<td>8f 2..1'</td>
<td>0.1/2,z [0,0,0]</td>
<td>0.1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,2z+1/2 [0,0,0]</td>
<td>1/2,0,2z [0,0,0]</td>
</tr>
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<td>8e -1'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
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<td>3/4,1/4,1/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4d 41'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<tr>
<td>4c 2.221'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
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<tr>
<td>4b 222.1'</td>
<td>0,0,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4a 222.1'</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
</tr>
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</table>

**Symmetry of Special Projections**

- **Along [0,0,1] p4mm1'**
  - \( a^* = \frac{(a - b)}{2} \)
  - \( b^* = \frac{(a + b)}{2} \)
  - Origin at 0,0,z

- **Along [1,0,0] p2mm1'**
  - \( a^* = \frac{b}{2} \)
  - \( b^* = c \)
  - Origin at x,0,1/4

- **Along [1,1,0] p2mm1'**
  - \( a^* = \frac{(a + b)}{2} \)
  - \( b^* = \frac{c}{2} \)
  - Origin at x,x,0
Origin at $\overline{4}12\overline{1}/c$, at $-1/4,1/4,-1/4$ from $\overline{1}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $\overline{1} (0,0,0)$
2. $2' 0,0,z$
3. $4' (0,0,1/2) 0,1/2,z$
4. $4' (0,0,1/2) 1/2,0,z$
5. $2' 0,y,1/4$
6. $2' x,0,1/4$
7. $2' (1/2,1/2,0) x,x,0$
8. $2' x,x+1/2,0$
9. $\overline{1} 1/4,1/4,1/4$
10. $n' (1/2,1/2,0) x,y,1/4$
11. $\overline{4}' 0,0,z$
12. $\overline{4}' 0,0,z$
13. $a (1/2,0,0) x,1/4,z$
14. $b (0,1/2,0) 1/4,y,z$
15. $c (0,0,1/2) x,x,1/4$
16. $c (0,0,1/2) x,x,z

133.3.1125 - 1 - 2341
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>.2'</td>
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<td>8</td>
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<td>22'</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>22'</td>
</tr>
</tbody>
</table>

### Coordinates

- (1) $x, y, z$ [u, v, w]
- (2) $x, y, z$ [u, v, w]
- (3) $y + 1/2, x + 1/2, z + 1/2$ [v, u, w]
- (4) $y + 1/2, x + 1/2, z + 1/2$ [v, u, w]
- (5) $x, y, z + 1/2$ [u, v, w]
- (6) $x, y, z + 1/2$ [u, v, w]
- (7) $y + 1/2, x + 1/2, z$ [v, u, w]
- (8) $y + 1/2, x + 1/2, z$ [v, u, w]
- (9) $x + 1/2, y + 1/2, z + 1/2$ [u, v, w]
- (10) $x + 1/2, y + 1/2, z + 1/2$ [u, v, w]
- (11) $y, x, z$ [v, u, w]
- (12) $y, x, z$ [v, u, w]
- (13) $x + 1/2, y + 1/2, z$ [u, v, w]
- (14) $x + 1/2, y + 1/2, z$ [u, v, w]
- (15) $y, x, z + 1/2$ [v, u, w]
- (16) $y, x, z + 1/2$ [v, u, w]
# Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>p4mm</th>
<th>p2a' 2mm</th>
<th>p2a' 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>a* = (a - b)/2  b* = (a + b)/2</td>
<td>a* = b/2    b* = c</td>
<td>a* = -c/2  b* = (-a + b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,z</td>
<td>Origin at x,1/4,1/4</td>
<td>Origin at x,x,1/4</td>
</tr>
</tbody>
</table>
**Origin** at $\bar{4}12_1/c$, at $-1/4,1/4,-1/4$ from $1$

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

**Symmetry Operations**

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
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<td>$1$</td>
</tr>
<tr>
<td>(2)</td>
<td>$2x,0,z$</td>
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<tr>
<td>(3)</td>
<td>$4'^{+}(0,0,1/2)\rightarrow 0,1/2,z$</td>
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<tr>
<td>(4)</td>
<td>$4'^{-}(1/2,1/2,1/2')$</td>
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<td>(5)</td>
<td>$2'0,y,1/4$</td>
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<tr>
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<td>$2'x,0,1/4$</td>
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<tr>
<td>(7)</td>
<td>$2(1/2,1/2,0)\rightarrow x,x,0$</td>
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<tr>
<td>(8)</td>
<td>$x,x+1/2,0$</td>
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<tr>
<td>(9)</td>
<td>$\bar{1}1/4,1/4,1/4$</td>
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<tr>
<td>(10)</td>
<td>$n(1/2,1/2,0)\rightarrow x,y,1/4$</td>
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<tr>
<td>(11)</td>
<td>$\bar{4}'\cdot 0,0,z; 0,0,0$</td>
</tr>
<tr>
<td>(12)</td>
<td>$\bar{4}'\cdot 0,0,z; 0,0,0$</td>
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<td>(13)</td>
<td>$a'(1/2,0,0)\rightarrow x,1/4,z$</td>
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<tr>
<td>(14)</td>
<td>$b'(0,1/2,0)\rightarrow 1/4,y,z$</td>
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<tr>
<td>(15)</td>
<td>$c(0,0,1/2)\rightarrow x,x,z$</td>
</tr>
<tr>
<td>(16)</td>
<td>$c(0,0,1/2)\rightarrow x,x,z$</td>
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</table>
**Generators selected**
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

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<th>Coordinates</th>
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<tr>
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<td>a 2</td>
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<td>1/2,0,3/4 [0,0,0]</td>
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</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] \( p_{\infty} 4mm \)
\[ a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \]
Origin at 0,0,z

Along [1,0,0] \( p2'mm' \)
\[ a^* = -c \quad b^* = \frac{b}{2} \]
Origin at x,0,1/4

Along [1,1,0] \( p_{2a'} 2m'm' \)
\[ a^* = -\frac{c}{2} \quad b^* = \frac{-(a + b)}{2} \]
Origin at x,x,0
Origin at $\overline{4}'12$_1'/c'$, at -1/4,1/4,-1/4 from $\overline{1}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) $z_0,0,0$

(3) $4'\cdot (0,0,1/2) 0,1/2,z$
(3) $4_z\cdot (1/2,1/2,1/2)'$

(4) $4'\cdot (0,0,1/2) 1/2,0,z$
(4) $4_z\cdot (1/2,1/2,1/2)'$

(5) 2 0,y,1/4
(5) $y_0,0,1/2$

(6) 2 0,y,1/4
(6) $z_0,0,1/2$

(7) 2' (1/2,1/2,0) x,x,0
(7) $2_{x'} (1/2,1/2,0)'$

(8) 2' x,x+1/2,0
(8) $2_{x'} (1/2,1/2,0)'$

(9) $\overline{4}'14,1/4,1/4$
(9) $\overline{1} 1/2,1/2,1/2$

(10) n (1/2,1/2,0) x,y,1/4
(10) $n_z 1/2,1/2,1/2$

(11) $\overline{4}'\cdot 0,0,z; 0,0,0$
(11) $\overline{4}_z\cdot (0,0,0)'$

(12) $\overline{4}'\cdot 0,0,z; 0,0,0$
(12) $\overline{4}_z\cdot (0,0,0)'$

(13) a (1/2,0,0) x,1/4,z
(13) $m_{x'} 1/2,1/2,0$

(14) b (0,1/2,0) 1/4,y,z
(14) $m_{xy} 1/2,1/2,0$

(15) $c' (0,0,1/2) x,x,z$
(15) $m_{xy} (0,0,1/2)'$

(16) $c' (0,0,1/2) x,x,z$
(16) $m_{xy} (0,0,1/2)'$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
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#### Coordinates

<table>
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<tr>
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<th>Coordinates</th>
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<tbody>
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<td>x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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</table>
Symmetry of Special Projections

Along $[0,0,1]$ $p_{12}$, $4m'm'$
\[a^* = (\mathbf{a} - \mathbf{b})/2 \quad b^* = (\mathbf{a} + \mathbf{b})/2\]
Origin at $\frac{1}{2},0,z$

Along $[1,0,0]$ $p_{2\alpha}$, $2m'm'$
\[a^* = -\mathbf{c} \quad b^* = \mathbf{b}/2\]
Origin at $x,0,\frac{1}{4}$

Along $[1,1,0]$ $p'2\text{mm}'$
\[a^* = (-\mathbf{a} + \mathbf{b})/2 \quad b^* = \mathbf{c}/2\]
Origin at $x,x,0$
Origin at $\overline{4}12/c$, at -$1/4,1/4,-1/4$ from $\overline{1}$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $1$
   
   $1 | 0,0,0$

2. $z$
   
   $z | 0,0,0$

3. $z'$
   
   $z | 1/2,1/2,0$

4. $x$
   
   $1/2,0,0$

5. $y$
   
   $0,1/2,0$

6. $z$
   
   $0,0,1/2$

7. $x$
   
   $x,x,0$

8. $y$
   
   $x,y,1/4$

9. $z$
   
   $x,x,z$

10. $x$
    
    $x,y,1/4$

11. $y$
    
    $1/2,1/2,0$

12. $z$
    
    $1/2,1/2,0$

13. $x$
    
    $1/2,0,0$

14. $y$
    
    $0,1/2,0$

15. $z$
    
    $0,0,1/2$

16. $x$
    
    $0,0,1/2$

17. $y$
    
    $0,0,0$

18. $z$
    
    $0,0,0$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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<tr>
<td>16</td>
<td>k</td>
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<tr>
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<td>j</td>
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<tr>
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Symmetry of Special Projections

Along [0,0,1] p4'mm'  
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] p2m'm'  
\[ a^* = \frac{b}{2} \quad b^* = c \]
Origin at x,0,1/4

Along [1,1,0] p2a* 2m'm'  
\[ a^* = \frac{-c}{2} \quad b^* = \frac{-(a + b)}{2} \]
Origin at x,x,0
**Origin** at \( \overline{4}12_1'/c' \), at \(-1/4,1/4,-1/4\) from \( \overline{1} \)

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

1. 1
2. \( 2^+ (0,0,0) \)
3. \( 4^+ (0,0,1/2) 0,1/2,z \)
4. \( 4^* (0,0,1/2) 1/2,0,z \)
5. \( 2' 0,y,1/4 \)
6. \( 2' x,0,1/4 \)
7. \( 2' (1/2,1/2,0) x,x,0 \)
8. \( 2' x,x+1/2,0 \)
9. \( \overline{1} 1/4,1/4,1/4 \)
10. \( n (1/2,1/2,0) x,y,1/4 \)
11. \( 4^* 0,0,z; 0,0,0 \)
12. \( 4^- 0,0,z; 0,0,0 \)
13. \( a' (1/2,0,0) x,1/4,z \)
14. \( b' (0,1/2,0) 1/4,y,z \)
15. \( c' (0,0,1/2) x,x,z \)
16. \( c' (0,0,1/2) x,x,z \)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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<th>Site Symmetry</th>
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<td>0,1/2,1/4 [0,0,w]</td>
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</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p\textsubscript{2}mm
\begin{align*}
a^* &= (a - b)/2 \\
b^* &= (a + b)/2
\end{align*}
Origin at 1/2,0,z

Along [1,0,0] p'2'mm
\begin{align*}
a^* &= -c \\
b^* &= b/2
\end{align*}
Origin at x,0,1/4

Along [1,1,0] p'2'mm
\begin{align*}
a^* &= -c/2 \\
b^* &= (-a + b)/2
\end{align*}
Origin at x,x,0
Origin at \( \bar{4}12_{1}/c' \), at \(-1/4, 1/4, -1/4\) from \( \bar{1} \)

Asymmetric unit \( \quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

1. \(1\)  \(1|0,0,0\)
2. \(2\)  \((0,0,z) \)  \(2|z|0,0,0\)
3. \(4'\)  \((0,0,1/2) \)  \(0,1/2,z\)  \(4_z|1/2,1/2,1/2'\)
4. \(4'\)  \((0,0,1/2) \)  \(1/2,0,z\)  \(4_{z'}|1/2,1/2,1/2'\)
5. \(2'\)  \(0,y,1/4\)  \(2_{y}|0,0,1/2'\)
6. \(2'\)  \(x,0,1/4\)  \(2_{x}|0,0,1/2'\)
7. \(2\)  \((1/2,1/2,0) \)  \(x,x,0\)  \(2_{x'}|1/2,1/2,0\)
8. \(2\)  \(x, x+1/2,0\)  \(2_{x'}|1/2,1/2,0\)
9. \(\bar{1}\)  \(1/4,1/4,1/4\)  \(1|1/2,1/2,1/2'\)
10. \(n'\)  \((1/2,1/2,0) \)  \(x,y,1/4\)  \(m_{y}|1/2,1/2,1/2'\)
11. \(\bar{4}^+\)  \((0,0,z) \)  \(0,0,0\)  \(\bar{4}_{z}|0,0,0\)
12. \(\bar{4}^-\)  \((0,0,z) \)  \(0,0,0\)  \(\bar{4}_{z'}|0,0,0\)
13. \(a\)  \((1/2,0,0) \)  \(x,1/4,z\)  \(m_{x}|1/2,1/2,0\)
14. \(b\)  \((0,1/2,0) \)  \(1/4,y,z\)  \(m_{y}|1/2,1/2,0\)
15. \(c'\)  \((0,0,1/2) \)  \(x,x,z\)  \(m_{x'}|0,0,1/2'\)
16. \(c'\)  \((0,0,1/2) \)  \(x,x,z\)  \(m_{x'}|0,0,1/2'\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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Symmetry of Special Projections

Along [0,0,1] p4'm'm
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] p2m'm'
\[ a^* = b/2 \quad b^* = c \]
Origin at x,1/4,1/4

Along [1,1,0] p2m'm'
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
**P4₁/n'b'c'**

133.9.1131

**4/m'm'**

P4₁/n'2/b'2/c'

**Tetragonal**

---

**Origin** at \( \overline{4}12_{1}/c' \), at \(-1/4,1/4,-1/4\) from \( \overline{1} \)

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

**Symmetry Operations**

1. \( 1 \)
2. \( 2; 0,0,z \)
3. \( 4^{+}; (0,0,1/2) 0,1/2,z \)
4. \( 4^{-}; (0,0,1/2) 1/2,0,z \)
5. \( 0,y,1/4 \)
6. \( x,0,1/4 \)
7. \( (1/2,1/2,0) x,x,0 \)
8. \( x,x+1/2,0 \)
9. \( 1/4,1/4,1/4 \)
10. \( (1/2,1/2,1/2) x,y,1/4 \)
11. \( (4) x,y,1/4 \)
12. \( (4) 0,0,0 \)
13. \( a' (1/2,0,0) x,1/4,z \)
14. \( b' (0,1/2,0) 1/4,y,z \)
15. \( c' (0,0,1/2) x,x,z \)
16. \( c' (0,0,1/2) x,x,z \)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, 
Wyckoff letter, 
Site Symmetry.

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<th>Multiplicity</th>
<th>Coordinates</th>
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<tr>
<td>(1) x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(2) x̅,y̅,z</td>
<td>[u̅,v̅,w]</td>
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<tr>
<td>(3) y+1/2,x+1/2,z+1/2</td>
<td>[v,u,w]</td>
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<td>(4) y+1/2,x+1/2,z+1/2</td>
<td>[v̅,u̅,w]</td>
</tr>
<tr>
<td>(5) x,y,z+1/2</td>
<td>[u,v,w]</td>
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<tr>
<td>(6) x,y,z+1/2</td>
<td>[u̅,v̅,w]</td>
</tr>
<tr>
<td>(7) y+1/2,x+1/2,z</td>
<td>[v,u,w]</td>
</tr>
<tr>
<td>(8) y+1/2,x+1/2,z</td>
<td>[v̅,u̅,w]</td>
</tr>
<tr>
<td>(9) x+1/2,y+1/2,z+1/2</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(10) x+1/2,y+1/2,z+1/2</td>
<td>[u̅,v̅,w]</td>
</tr>
<tr>
<td>(11) x̅,x̅,z</td>
<td>[v̅,u̅,w]</td>
</tr>
<tr>
<td>(12) y̅,x̅,z</td>
<td>[v,u̅,w]</td>
</tr>
<tr>
<td>(13) x+1/2,y+1/2,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(14) x+1/2,y+1/2,z</td>
<td>[u̅,v̅,w]</td>
</tr>
<tr>
<td>(15) y̅,x̅,z+1/2</td>
<td>[v,u̅,w]</td>
</tr>
<tr>
<td>(16) y̅,x̅,z+1/2</td>
<td>[v,u̅,w]</td>
</tr>
</tbody>
</table>

8     j  .2  x,x+1/2,0 [u,u,0]  x̅,x+1/2,0 [u̅,u,0]  x̅,x+1/2,1/2 [u,u,0]  x̅,x+1/2,1/2 [u̅,u,0]  x+1/2,x,1/2 [u,u,0]  x+1/2,x,1/2 [u̅,u,0]  x+1/2,x,0 [u,u,0]  x+1/2,x,0 [u̅,u,0]

8     i  .2  x,0,3/4 [u,0,0]  x,0,3/4 [u,0,0]  1/2,x+1/2,1/4 [0,u,0]  1/2,x+1/2,1/4 [0,u,0]  x+1/2,1/2,3/4 [u̅,0,0]  x+1/2,1/2,3/4 [u̅,0,0]  0,x,1/4 [0,u,0]  0,x,1/4 [0,u,0]

8     h  .2  x,0,1/4 [u,0,0]  x̅,0,1/4 [u̅,0,0]  1/2,x+1/2,3/4 [0,u,0]  1/2,x+1/2,3/4 [0,u,0]  x+1/2,1/2,1/4 [u̅,0,0]  x+1/2,1/2,1/4 [u̅,0,0]  0,x,3/4 [0,u,0]  0,x,3/4 [0,u,0]

8     g  2.. 0,0,z [0,0,w]  1/2,1/2,z+1/2 [0,0,w]  0,0,z+1/2 [0,0,w]  1/2,1/2,z [0,0,w]  1/2,1/2,z [0,0,0,w]  0,0,z [0,0,w]  1/2,1/2,z+1/2 [0,0,w]  0,0,z+1/2 [0,0,w]

8     f  2.. 0,1/2,z [0,0,w]  0,1/2,z+1/2 [0,0,w]  0,1/2,z+1/2 [0,0,w]  0,1/2,z [0,0,w]  1/2,0,1/2 [0,0,w,w]  1/2,0,1/2 [0,0,w,w]  1/2,0,z [0,0,w]  1/2,0,z [0,0,w]

8     e  41  1/4,1/4,1/4 [0,0,0]  3/4,3/4,1/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  3/4,1/4,3/4 [0,0,0]  1/4,3/4,1/4 [0,0,0]  3/4,3/4,1/4 [0,0,0]  3/4,3/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]

4     d  41  0,0,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]  0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]  0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]

4     c  22. 0,1/2,0 [0,0,0]  0,1/2,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]  1/2,0,0 [0,0,0]  1/2,0,0 [0,0,0]  1/2,0,0 [0,0,0]

4     b  222. 0,0,1/4 [0,0,0]  1/2,1/2,3/4 [0,0,0]  1/2,1/2,3/4 [0,0,0]  0,0,3/4 [0,0,0]  0,0,3/4 [0,0,0]  0,0,3/4 [0,0,0]  0,0,3/4 [0,0,0]  0,0,3/4 [0,0,0]

4     a  222. 0,1/2,1/4 [0,0,0]  0,1/2,3/4 [0,0,0]  0,1/2,3/4 [0,0,0]  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]  1/2,0,0 [0,0,0]  1/2,0,0 [0,0,0]  1/2,0,0 [0,0,0]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Equations</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1] p4m'</td>
<td>$a^* = (a - b)/2$</td>
<td>0,0,z</td>
</tr>
<tr>
<td></td>
<td>$b^* = (a + b)/2$</td>
<td></td>
</tr>
<tr>
<td>[1,0,0] p2m'</td>
<td>$a^* = b/2$</td>
<td>x,0,1/4</td>
</tr>
<tr>
<td></td>
<td>$b^* = c$</td>
<td></td>
</tr>
<tr>
<td>[1,1,0] p2m'</td>
<td>$a^* = (a + b)/2$</td>
<td>x,x,0</td>
</tr>
<tr>
<td></td>
<td>$b^* = c/2$</td>
<td></td>
</tr>
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</table>
P4$_2$/nnm
134.1.1132

4/mmm
P4$_2$/n2/n2/m

Tetragonal

Origin at $\bar{4}2m$ at $-1/4,1/4,-1/4$ from center ($2/m$)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4; \quad x < y; \quad y \leq 1-x$

Symmetry Operations

(1) 1
   (1 0,0,0)

(5) 2 0,y,0
    (2_y 0,0,0)

(9) $\bar{1}$ 1/4,1/4,1/4
    (1 1/2,1/2,1/2)

(13) n (1/2,0,1/2) x,1/4,z
     (m_y 1/2,1/2,1/2)

(2) 2 0,0,z
    (2_z 0,0,0)

(6) 2 x,0,0
    (2_x 0,0,0)

(10) n (1/2,1/2,0) x,y,1/4
     (m_z 1/2,1/2,1/2)

(14) n (0,1/2,1/2) 1/4,y,z
     (m_x 1/2,1/2,1/2)

(3) $4^+$ (0,0,1/2) 0,1/2,z
    ($4_z^{+}$ 1/2,1/2,1/2)

(7) 2 (1/2,1/2,0) x,x,1/4
    ($2_{xy}$ 1/2,1/2,1/2)

(11) $\bar{4}^+$ 0,0,z; 0,0,0
     ($\bar{4}_z$ 0,0,0)

(15) m x,x,z
     (m_x 0,0,0)

(4) $4^-$ (0,0,1/2) 1/2,0,z
    ($4_z^{-}$ 1/2,1/2,1/2)

(8) 2 x,x+1/2,1/4
    ($2_{xy}$ 1/2,1/2,1/2)

(12) $\bar{4}^-$ 0,0,z; 0,0,0
     ($\bar{4}_z$ 0,0,0)

(16) m x,x,z
     (m_x 0,0,0)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

- **Multiplicity**, **Wyckoff letter**, **Site Symmetry.**

<table>
<thead>
<tr>
<th>N</th>
<th>Wyckoff Letter</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>n</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y+1/2, x+1/2, z+1/2 [v, u, w]</td>
<td>(4) y+1/2, x+1/2, z+1/2 [v, u, w]</td>
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<td>(5) x, y, z [u, v, w]</td>
<td>(6) x, y, z [u, v, w]</td>
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<td></td>
<td>(7) y+1/2, x+1/2, z+1/2 [v, u, w]</td>
<td>(8) y+1/2, x+1/2, z+1/2 [v, u, w]</td>
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<tr>
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<td>(9) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
<td>(10) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
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<td>(11) y, x, z [v, u, w]</td>
<td>(12) y, x, z [v, u, w]</td>
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<td></td>
<td>(13) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
<td>(14) x+1/2, y+1/2, z+1/2 [u, v, w]</td>
</tr>
<tr>
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<td>(15) y, x, z [v, u, w]</td>
<td>(16) y, x, z [v, u, w]</td>
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<td>8</td>
<td>m</td>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
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<td>.m</td>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
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<tr>
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<td>x,x+1/2,3/4 [u,u,0]</td>
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<td>x,x+1/2,1/4 [u,u,0]</td>
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<td>x,x+1/2,1/4 [u,u,0]</td>
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<td>x,0, 1/2 [u,0,0]</td>
<td>x,0, 1/2 [u,0,0]</td>
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<td>x,0, 1/2 [u,0,0]</td>
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<tr>
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<td>i</td>
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<td>x,0, 0 [u,0,0]</td>
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<td>x,0, 0 [u,0,0]</td>
<td>x,0, 0 [u,0,0]</td>
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<tr>
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<td>h</td>
<td>0,1/2, z [0,0,w]</td>
<td>0,1/2, z+1/2 [0,0,w]</td>
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<td>2..</td>
<td>0,1/2, z+1/2 [0,0,w]</td>
<td>1/2,0, z [0,0,w]</td>
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<tr>
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<td>g</td>
<td>0,0, z [0,0,0]</td>
<td>0,0, z [0,0,0]</td>
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<td>0,0, z [0,0,0]</td>
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<tr>
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<td>1/4,1/4,1/4 [u,u,0]</td>
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<td>1/4,1/4,1/4 [u,u,0]</td>
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<tr>
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<td>d</td>
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<td>0,1/2,3/4 [0,0,0]</td>
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<td>0,1/2,3/4 [0,0,0]</td>
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</table>
4 c 222. 0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,0 [0,0,0]
2 b 42m 0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]
2 a 42m 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p, 4m'm'  
\[ a^* = \frac{(a - b)}{2}, \quad b^* = \frac{(a + b)}{2} \]
Origin at 1/2,0,z

Along [1,0,0] c, 2m'm'  
\[ a^* = b, \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p2mm1'  
\[ a^* = \frac{(-a + b)}{2}, \quad b^* = c \]
Origin at x,x,1/4
Origin at $\overline{4}2m1'$ at $-1/4,1/4,-1/4$ from center ($2/m1'$)

Asymmetric unit

$$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4; \quad x < y; \quad y \leq 1-x$$

Symmetry Operations

For $1 +$ set

(1) $1$
(2) $2$ $0,0,z$
(3) $4^+ (0,0,1/2)$ $0,1/2,z$
(4) $4' (0,0,1/2)$ $1/2,0,z$

(5) $2$ $0,y,0$
(6) $2$ $x,0,0$
(7) $2$ $(1/2,1/2,0)$ $x,x,1/4$
(8) $2$ $x,x+1/2,1/4$

(9) $\overline{1}$ $1/4,1/4,1/4$
(10) $n$ $(1/2,1/2,0)$ $x,y,1/4$
(11) $\overline{4}^+$ $0,0,z; 0,0,0$
(12) $\overline{4}'^- 0,0,z; 0,0,0$

(13) $n$ $(1/2,0,1/2)$ $x,1/4,z$
(14) $n$ $(0,1/2,1/2)$ $1/4,y,z$
(15) $m$ $x,x,z$
(16) $m$ $x,x,z$
For \(1'\) + set

\[
\begin{align*}
(1) \ 1' & \quad (2) \ 2' & \quad (3) \ 4' & \quad (4) \ 4' \\
(1', 0, 0, 0) & \quad (2, 0, 0, 0) & \quad (0, 0, 1/2, 0) & \quad (0, 0, 1/2, 0) \\
(2, 0, 0, 0) & \quad (4, 1/2, 1/2, 1/2) & \quad (4, 1/2, 1/2, 1/2) & \quad (4, 1/2, 1/2, 1/2)
\end{align*}
\]

\[
\begin{align*}
(5) \ 2' & \quad (6) \ 2' & \quad (7) \ 2' & \quad (8) \ 2' \\
0, y, 0 & \quad x, 0, 0 & \quad (1/2, 1, 2, 0) & \quad (1/2, x + 1, 1/2, 1/4) \\
(2, 0, 0, 0) & \quad (2, 0, 0, 0) & \quad (2, 1/2, 1, 2, 1/2) & \quad (2, 1/2, 1, 2, 1/2)
\end{align*}
\]

\[
\begin{align*}
(9) \ T' & \quad (10) \ n' & \quad (11) \ n' & \quad (12) \ n' \\
1/4, 1/4, 1/4 & \quad (1/2, 1, 2, 0) & \quad 0, 0, 0; 0, 0, 0 & \quad 0, 0, 0; 0, 0, 0 \\
(1/2, 1, 2, 1/2) & \quad (m, 1/2, 1, 1/2) & \quad (4, 0, 0) & \quad (4, 0, 0)
\end{align*}
\]

\[
\begin{align*}
(13) \ n' & \quad (14) \ n' & \quad (15) \ m' & \quad (16) \ m' \\
(1/2, 0, 1/2) & \quad (0, 1/2, 1/2) & \quad (1/2, 0, 1/2) & \quad (0, 1/2, 1/2) \\
(1/2, 1/2, 1/2) & \quad (1/2, 1/2, 1/2) & \quad (1/2, 1/2, 1/2) & \quad (1/2, 1/2, 1/2)
\end{align*}
\]

Generators selected

\[(1); \ t(1, 0, 0); \ t(0, 1, 0); \ t(0, 0, 1); \ (2); \ (3); \ (5); \ (9); \ 1'.\]

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>n</td>
<td>11'</td>
</tr>
<tr>
<td>16</td>
<td>m</td>
<td>.m1'</td>
</tr>
<tr>
<td>8</td>
<td>l</td>
<td>.21'</td>
</tr>
<tr>
<td>8</td>
<td>k</td>
<td>.21'</td>
</tr>
<tr>
<td>8</td>
<td>j</td>
<td>.21'</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
& (1) \ x, y, z [0, 0, 0] \quad (2) \ x, y, z [0, 0, 0] \\
& (3) \ y+1/2, x+1/2, z+1/2 [0, 0, 0] \quad (4) \ y+1/2, x+1/2, z+1/2 [0, 0, 0] \\
& (5) \ x, y, z [0, 0, 0] \quad (6) \ x, y, z [0, 0, 0] \\
& (7) \ y+1/2, x+1/2, z+1/2 [0, 0, 0] \quad (8) \ y+1/2, x+1/2, z+1/2 [0, 0, 0] \\
& (9) \ x+1/2, y+1/2, z+1/2 [0, 0, 0] \quad (10) \ x+1/2, y+1/2, z+1/2 [0, 0, 0] \\
& (11) \ y, x, z [0, 0, 0] \quad (12) \ y, x, z [0, 0, 0] \\
& (13) \ x+1/2, y+1/2, z+1/2 [0, 0, 0] \quad (14) \ x+1/2, y+1/2, z+1/2 [0, 0, 0] \\
& (15) \ x, x, z [0, 0, 0] \quad (16) \ x, x, z [0, 0, 0] \\
\end{align*}
\]
Symmetry of Special Projections

Along [0,0,1] p4mm1'  
\( a^* = (a - b)/2 \quad b^* = (a + b)/2 \)
Origin at 0,0,z

Along [1,0,0] c2mm1'  
\( a^* = b \quad b^* = c \)
Origin at x,0,0

Along [1,1,0] p2mm1'  
\( a^* = (-a + b)/2 \quad b^* = c \)
Origin at x,x,1/4
**Origin** at $\overline{4}^* 2'm$ at $-1/4,1/4,-1/4$ from center ($2'm$)

**Asymmetric unit**

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4; \quad x < y; \quad y \leq 1-x$

**Symmetry Operations**

1. (1) $1$
   - $(1|0,0,0)$
2. (2) $2' \ 0,0,z$
   - $(2_z|0,0,0)$
3. (3) $4'^+ (0,0,1/2) \ 0,1/2,z$
   - $(4_z|1/2,1/2,1/2)$
4. (4) $4' (0,0,1/2) \ 1/2,0,z$
   - $(4_z^{-1}|1/2,1/2,1/2)$
5. (5) $2' \ 0,y,0$
   - $(2_z|0,0,0)'$
6. (6) $2' \ x,0,0$
   - $(2_z|0,0,0)'$
7. (7) $2' (1/2,1/2,0) \ x,x,1/4$
   - $(2_{xy}|1/2,1/2,1/2)'$
8. (8) $2' x,x+1/2,1/4$
   - $(2_{xy}|1/2,1/2,1/2)'$
9. (9) $\overline{1}' \ 1/4,1/4,1/4$
   - $(1|1/2,1/2,1/2)'$
10. (10) $n' (1/2,1/2,0) \ x,y,1/4$
    - $(m_z|1/2,1/2,1/2)'$
11. (11) $\overline{4}'^+ \ 0,0,z; \ 0,0,0$
    - $(\overline{4}_z|0,0,0)'$
12. (12) $\overline{4}' \ 0,0,z; \ 0,0,0$
    - $(\overline{4}_z^{-1}|0,0,0)'$
13. (13) $n (1/2,0,1/2) \ x,1/4,z$
    - $(m_y|1/2,1/2,1/2)$
14. (14) $n (0,1/2,1/2) \ 1/4,y,z$
    - $(m_y|1/2,1/2,1/2)$
15. (15) $m \ x,x,z$
    - $(m_{xy}|0,0,0)$
16. (16) $m \ x,x,z$
    - $(m_{xy}|0,0,0)$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
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<td>(1) x,y,z [u,v,w]</td>
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<td>x,y,z [u,u,0]</td>
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<td>0,1/2,1/4 [0,0,w]</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] p4mm
\[ \mathbf{a}^* = \frac{(\mathbf{a} - \mathbf{b})}{2} \quad \mathbf{b}^* = \frac{(\mathbf{a} + \mathbf{b})}{2} \]
Origin at 0,0,z

Along [1,0,0] \( c_p \) 2'mm'
\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at x,0,0

Along [1,1,0] p2mm1'
\[ \mathbf{a}^* = \frac{(-\mathbf{a} + \mathbf{b})}{2} \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,1/4
Origin at $\bar{4} \bar{2} \bar{m}$ at -1/4, 1/4, -1/4 from center (2/m)

Asymmetric unit

$x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4; \quad x < y; \quad y \leq 1-x$

Symmetry Operations

1. 1
   
2. $2 \cdot 0,0,z$
   $(2_z \cdot 0,0,0)$
   
3. $4' \cdot (0,0,1/2) \quad 0,1/2,z$
   $(4_z \cdot 1/2,1/2,1/2)'$
   
4. $4' \cdot (0,0,1/2) \quad 1/2,0,z$
   $(4_z \cdot 1/2,1/2,1/2)'$
   
5. $2' \cdot 0,y,0$
   $(2_z \cdot 0,0,0)'$
   
6. $2' \cdot x,0,0$
   $(2_x \cdot 0,0,0)'$
   
7. $2 \cdot (1/2,1/2,0) \quad x,x,1/4$
   $(2_{xy} \cdot 1/2,1/2,1/2)$
   
8. $2 \cdot x,x+1/2,1/4$
   $(2_{xy} \cdot 1/2,1/2,1/2)$
   
9. $T \cdot 1/4,1/4,1/4$
   $(T \cdot 1/2,1/2,1/2)$
   
10. $n \cdot (1/2,1/2,0) \quad x,y,1/4$
    $(m_x \cdot 1/2,1/2,1/2)$
    
11. $\bar{4} \cdot -0,0,z; \quad 0,0,0$
    $(\bar{4}_z \cdot 0,0,0)'$
    
12. $\bar{4} \cdot -0,0,z; \quad 0,0,0$
    $(\bar{4}_z \cdot 0,0,0)'$
    
13. $n' \cdot (1/2,0,1/2) \quad x,1/4,z$
    $(m_y \cdot 1/2,1/2,1/2)'$
    
14. $n' \cdot (0,1/2,1/2) \quad 1/4,y,z$
    $(m_{xy} \cdot 0,0,0)$
    
15. $m \cdot x,x,z$
    $(m_{xy} \cdot 0,0,0)$
    
16. $m \cdot x,x,z$
    $(m_{xy} \cdot 0,0,0)$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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</tr>
<tr>
<td>16 n 1</td>
<td>( (1) x,y,z \ [u,v,w] ) ( (2) \tilde{x},\tilde{y},\tilde{z} \ [\tilde{u},\tilde{v},w] )</td>
</tr>
<tr>
<td></td>
<td>( (3) \tilde{y} + 1/2, x+1/2, z+1/2 \ [v,u,w] ) ( (4) y+1/2, x+1/2, z+1/2 \ [v,u,w] )</td>
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<tr>
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<td>( (5) \tilde{x},\tilde{y},\tilde{z} \ [u,\tilde{v},w] ) ( (6) x,\tilde{y},\tilde{z} \ [u,v,w] )</td>
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<tr>
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<td>( (7) y+1/2, x+1/2, z+1/2 \ [v,u,w] ) ( (8) y+1/2, x+1/2, z+1/2 \ [v,u,\tilde{w}] )</td>
</tr>
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<td>( (9) x+1/2, y+1/2, z+1/2 \ [u,v,w] ) ( (10) x+1/2, y+1/2, z+1/2 \ [u,v,w] )</td>
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<td>( (11) \tilde{x},\tilde{y},\tilde{z} \ [v,u,w] ) ( (12) \tilde{y},x,\tilde{z} \ [v,u,\tilde{w}] )</td>
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<td>( (13) x+1/2, \tilde{y} + 1/2, z+1/2 \ [u,\tilde{v},w] ) ( (14) x+1/2, y+1/2, z+1/2 \ [u,v,w] )</td>
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<td>( (15) \tilde{x},\tilde{y},\tilde{z} \ [v,\tilde{u},w] ) ( (16) y,x,z \ [\tilde{v},u,w] )</td>
</tr>
<tr>
<td>8 m .m</td>
<td>( x,x,z \ [u,u,0] ) ( x,x,z \ [\tilde{u},u,0] ) ( \tilde{x}+1/2, x+1/2, z+1/2 \ [u,u,0] ) ( x+1/2, x+1/2, z+1/2 \ [\tilde{u},u,0] )</td>
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<td>( \tilde{x},x,z \ [u,u,0] ) ( x,x,z \ [u,u,0] ) ( x+1/2, x+1/2, z+1/2 \ [\tilde{u},u,0] ) ( \tilde{x}+1/2, x+1/2, z+1/2 \ [u,u,0] )</td>
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<tr>
<td>8 l .2</td>
<td>( x,x+1/2,3/4 \ [u,u,0] ) ( x,x+1/2,3/4 \ [u,u,0] ) ( \tilde{x},x+1/2,1/4 \ [\tilde{u},u,0] ) ( x+1/2, x+1/2,1/4 \ [\tilde{u},u,0] )</td>
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<td>( x,x+1/2,3/4 \ [u,u,0] ) ( x,x+1/2,3/4 \ [u,u,0] ) ( \tilde{x},x+1/2,1/4 \ [\tilde{u},u,0] ) ( x+1/2, x+1/2,1/4 \ [\tilde{u},u,0] )</td>
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<td>8 k .2</td>
<td>( x,x+1/2,1/4 \ [u,u,0] ) ( x,x+1/2,1/4 \ [u,u,0] ) ( \tilde{x},x+1/2,3/4 \ [\tilde{u},u,0] ) ( x+1/2, x+1/2,3/4 \ [\tilde{u},u,0] )</td>
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<td>( x,x+1/2,1/4 \ [u,u,0] ) ( x,x+1/2,1/4 \ [u,u,0] ) ( \tilde{x},x+1/2,3/4 \ [\tilde{u},u,0] ) ( x+1/2, x+1/2,3/4 \ [\tilde{u},u,0] )</td>
</tr>
<tr>
<td>8 j .2'</td>
<td>( x,0,1/2 \ [0,v,w] ) ( x,0,1/2 \ [0,v,w] ) ( \tilde{x},0,1/2 \ [0,\tilde{v},w] ) ( 1/2, x+1/2,0 \ [v,0,w] )</td>
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<td>( x,0,1/2 \ [0,v,w] ) ( x,0,1/2 \ [0,v,w] ) ( \tilde{x},0,1/2 \ [0,\tilde{v},w] ) ( 1/2, x+1/2,0 \ [v,0,w] )</td>
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<tr>
<td>8 i .2'</td>
<td>( x,0,0 \ [0,v,w] ) ( x,0,0 \ [0,\tilde{v},w] ) ( x+1/2,1/2,1/2 \ [0,\tilde{v},w] ) ( 1/2, x+1/2,1/2 \ [v,0,w] )</td>
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<tr>
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<td>( x,0,0 \ [0,v,w] ) ( x,0,0 \ [0,\tilde{v},w] ) ( x+1/2,1/2,1/2 \ [0,\tilde{v},w] ) ( 1/2, x+1/2,1/2 \ [v,0,w] )</td>
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<tr>
<td>8 h 2.</td>
<td>( 0,1/2,z \ [0,0,w] ) ( 0,1/2,z+1/2 \ [0,0,w] ) ( 0,1/2,z \ [0,0,w] ) ( 0,1/2,z+1/2 \ [0,0,w] )</td>
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<td>( 0,1/2,z \ [0,0,w] ) ( 0,1/2,z+1/2 \ [0,0,w] ) ( 0,1/2,z \ [0,0,w] ) ( 0,1/2,z+1/2 \ [0,0,w] )</td>
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<td>( 0,0,z \ [0,0,0] ) ( 1/2,1/2,z+1/2 \ [0,0,0] ) ( 0,0,z \ [0,0,0] ) ( 1/2,1/2,z+1/2 \ [0,0,0] )</td>
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<td>4 f .2/m</td>
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<tr>
<td>4 e .2/m</td>
<td>( 1/4,1/4,1/4 \ [\tilde{u},u,0] ) ( 3/4,3/4,1/4 \ [u,u,0] ) ( 1/4,3/4,3/4 \ [u,u,0] ) ( 3/4,1/4,3/4 \ [\tilde{u},u,0] )</td>
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4 c 22'2'. 0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,0 [0,0,0]
2 b 4'2'm 0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0]
2 a 4'2'm 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p₄, 4mm
\[ \mathbf{a}^* = \frac{(\mathbf{a} - \mathbf{b})}{2} \quad \mathbf{b}^* = \frac{(\mathbf{a} + \mathbf{b})}{2} \]
Origin at 0,0,z

Along [1,0,0] c₂'mm'
\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at x,0,0

Along [1,1,0] p₂mm¹'
\[ \mathbf{a}^* = \frac{(-\mathbf{a} + \mathbf{b})}{2} \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,1/4
Origin at $\overline{4}'2m'$ at $-1/4, 1/4, -1/4$ from center ($2'm'$)

Asymmetric unit

\[
0 ≤ x ≤ 1/2; \quad 0 ≤ y ≤ 1; \quad 0 ≤ z ≤ 1/4; \quad x ≤ y; \quad y ≤ 1-x
\]

Symmetry Operations

1. \(1\)
   \((1|0,0,0)\)

2. \(2\)
   \((0,0,z)\)
   \((2_z|0,0,0)\)

3. \(4'\)
   \((0,0,1/2)\)
   \(0,1/2,z\)
   \((4_z|1/2,1/2,1/2)\)

4. \(4'\)
   \((0,0,1/2)\)
   \(1/2,0,z\)
   \((4_z|1/2,1/2,1/2)\)

5. \(2\)
   \(0,y,0\)
   \((2_y|0,0,0)\)

6. \(2\)
   \(x,0,0\)
   \((2_x|0,0,0)\)

7. \(2'\)
   \((1/2,1/2,0)\)
   \(x,x,1/4\)
   \((2_x|1/2,1/2,1/2)\)

8. \(2'\)
   \(x,x+1/2,1/4\)
   \((2_x|1/2,1/2,1/2)\)

9. \(1/4,1/4,1/4\)
   \((1|1/2,1/2,1/2)\)

10. \(n\)
    \((1/2,1/2,0)\)
    \(x,y,1/4\)
    \((m_x|1/2,1/2,1/2)\)

11. \(\overline{4}'\)
    \(0,0,z\)
    \(0,0,0\)
    \((\overline{4}_z|0,0,0)\)

12. \(\overline{4}'\)
    \(0,0,z\)
    \(0,0,0\)
    \((\overline{4}_z|0,0,0)\)

13. \(n\)
    \((1/2,0,1/2)\)
    \(x,1/4,z\)
    \((m_y|1/2,1/2,1/2)\)

14. \(n\)
    \((0,1/2,1/2)\)
    \(1/4,y,z\)
    \((m_y|1/2,1/2,1/2)\)

15. \(m'\)
    \(x,x,z\)
    \((m_x|0,0,0)\)

16. \(m'\)
    \(x,x,z\)
    \((m_y|0,0,0)\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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<td>(11) y,x,z [v,u,w]</td>
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Continued

| 4 | c | 222. | 0,1/2,0 [0,0,0] | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,0,0 [0,0,0] |
| 2 | b | 4'2m' | 0,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 2 | a | 4'2m' | 0,0,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p, 4m'm'

\[ {\mathbf{a}}^* = (\mathbf{a} - \mathbf{b})/2 \]
\[ {\mathbf{b}}^* = (\mathbf{a} + \mathbf{b})/2 \]

Origin at 0,0,z

Along [1,0,0] c, 2m'm'

\[ {\mathbf{a}}^* = \mathbf{b} \]
\[ {\mathbf{b}}^* = \mathbf{c} \]

Origin at 0,0,0

Along [1,1,0] p2mm'

\[ {\mathbf{a}}^* = -\mathbf{c} \]
\[ {\mathbf{b}}^* = (-\mathbf{a} + \mathbf{b})/2 \]

Origin at x,x,1/4
Origin at $\overline{4}2m$ at -1/4, 1/4, -1/4 from center (2/m)

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/4; x ≤ y; y ≤ 1-x

Symmetry Operations

1. 1 
   (1 0 0 0)
2. 2 0,0,z
   (2z 0 0 0)
3. $4^+$ (0,0,1/2) 0,1/2,z
   (4z 1/2,1/2,1/2)' 
4. $4^-$ (0,0,1/2) 1/2,0,z
   (4z -1/2,1/2,1/2)'
5. 2 0,y,0
   (2y 0 0 0)
6. 2 x,0,0
   (2z 0 0 0)
7. 2' (1/2,1/2,0) x,x,1/4
   (2xy 1/2,1/2,1/2)'
8. 2' x,x+1/2,1/4
   (2xy 1/2,1/2,1/2)'
9. $\overline{3}$ 1/4, 1/4, 1/4
   (1 1/2,1/2,1/2)'
10. $\overline{3}'$ (1/2,1/2,0) x,y,1/4
    (mz 1/2,1/2,1/2)'
11. $\overline{4}^+$ 0,0,z; 0,0,0
    (4z 0,0,0)
12. $\overline{4}^-$ 0,0,z; 0,0,0
    (4z -1/0,0,0)
13. $n'$ (1/2,0,1/2) x,1/4,z
    (mz 1/2,1/2,1/2)'
14. $n'$ (0,1/2,1/2) 1/4,y,z
    (mz 1/2,1/2,1/2)'
15. m x,x,z
    (mx 0,0,0)
16. m x,x,z
    (mx 0,0,0)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
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<td>(1) x,y,z [u,v,w]</td>
<td>(2) x̅,y,z [u̅,v̅,w]</td>
</tr>
<tr>
<td>(3) y̅+1/2,x+1/2,z+1/2 [v̅,u̅,w]</td>
<td>(4) y+1/2,x̅+1/2,z+1/2 [v̅,u̅,w]</td>
</tr>
<tr>
<td>(5) x̅,y,z [u̅,v̅,w]</td>
<td>(6) x̅,y,z [u̅,v̅,w]</td>
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<tr>
<td>(7) y+1/2,x+1/2,z+1/2 [v̅,u̅,w]</td>
<td>(8) y+1/2,x̅+1/2,z+1/2 [v̅,u̅,w]</td>
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<tr>
<td>(9) x̅+1/2,y+1/2,z+1/2 [u̅,v̅,w]</td>
<td>(10) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td>(11) x̅,y,z [v̅,u̅,w]</td>
<td>(12) y,x,z [v,u,w]</td>
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<tr>
<td>(13) x+1/2,y̅+1/2,z+1/2 [u̅,v,w]</td>
<td>(14) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
<td>(15) y̅,x,z [v,u,w]</td>
<td>(16) y,x,z [v,u,w]</td>
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</table>

8 m ..m
x,x,z [u,u,0] x̅,x,z [u̅,u̅,0] x+1/2,x+1/2,z+1/2 [u,u,0] x+1/2,x+1/2,z+1/2 [u,u,0] x+1/2,x+1/2,z+1/2 [u,u,0] x+1/2,x+1/2,z+1/2 [u,u,0]

8 l ..2'
x,x+1/2,3/4 [u,u,w] x̅,x+1/2,3/4 [u̅,u̅,w] x̅,x+1/2,1/4 [u̅,u̅,w] x+1/2,x̅+1/2,1/4 [u̅,u̅,w] x+1/2,x+1/2,1/4 [u,u,0] x+1/2,x+1/2,1/4 [u,u,0] x+1/2,x+1/2,1/4 [u,u,0] x+1/2,x+1/2,1/4 [u,u,0]

8 k ..2'
x,x+1/2,1/4 [u,u,w] x̅,x+1/2,1/4 [u̅,u̅,w] x̅,x+1/2,3/4 [u̅,u̅,w] x+1/2,x̅+1/2,3/4 [u̅,u̅,w] x+1/2,x+1/2,3/4 [u,u,0] x+1/2,x+1/2,3/4 [u,u,0] x+1/2,x+1/2,3/4 [u,u,0] x+1/2,x+1/2,3/4 [u,u,0]

8 j ..2
x,0,1/2 [u,u,0] x̅,0,1/2 [u̅,u̅,0] 1/2,x+1/2,0 [0,u,0] 1/2,x+1/2,0 [0,u,0] 1/2,x+1/2,0 [0,u,0] 1/2,x+1/2,0 [0,u,0] 1/2,x+1/2,0 [0,u,0] 1/2,x+1/2,0 [0,u,0]

8 i ..2
x,0,0 [u,u,0] x̅,0,0 [u̅,u̅,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,x+1/2,1/2 [0,u,0]

8 h 2..
0,1/2,z [0,0,w] 0,1/2,z+1/2 [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z+1/2 [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z+1/2 [0,0,w] 0,1/2,z [0,0,w] 0,1/2,z+1/2 [0,0,w]

1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w]

4 g 2mm
0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0]

4 f ..2'm
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4 e ..2'm
1/4,1/4,1/4 [0,0,0] 3/4,3/4,1/4 [0,0,0] 1/4,3/4,3/4 [0,0,0] 3/4,1/4,3/4 [0,0,0] 3/4,1/4,3/4 [0,0,0] 1/4,3/4,1/4 [0,0,0] 3/4,1/4,3/4 [0,0,0] 1/4,3/4,1/4 [0,0,0]

4 d 222'
0,1/2,1/4 [0,0,w] 0,1/2,3/4 [0,0,w] 0,1/2,1/4 [0,0,w] 0,1/2,3/4 [0,0,w] 0,1/2,1/4 [0,0,w] 0,1/2,3/4 [0,0,w] 0,1/2,1/4 [0,0,w] 0,1/2,3/4 [0,0,w]
Symmetry of Special Projections

Along [0,0,1] p4'2/m
\[a^* = (a - b)/2, \quad b^* = (a + b)/2\]
Origin at 0,0,z

Along [1,0,0] c2/m'm'
\[a^* = b, \quad b^* = c\]
Origin at x,0,0

Along [1,1,0] p2m1'
\[a^* = (-a + b)/2, \quad b^* = c\]
Origin at x,x,1/4
Origin at $\bar{4}2'm'$ at -1/4,1/4,-1/4 from center ($2'm'$)

Asymmetric unit:

$$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4; \quad x < y; \quad y \leq 1-x$$

Symmetry Operations:

1. $1$
   
   (1) $0,0,0$

2. $2' \cdot 0,z$  
   (2) $2'? \cdot 0,0,0$
   
3. $4' \cdot (0,0,1/2)$  
   (3) $4' \cdot 0,1/2,z$
   
4. $4' \cdot (0,0,1/2)$  
   (4) $4' \cdot 1/2,1/2,1/2$

5. $2' \cdot 0,y,0$
   (5) $2' \cdot (0,0,0)'$

6. $2' \cdot x,0,0$
   (6) $2' \cdot x,0,0$

7. $2' \cdot (1/2,1/2,0)$  
   (7) $2' \cdot (1/2,1/2,0)$
   
8. $2' \cdot x+1/2,1/2$  
   (8) $2' \cdot x+1/2,1/2$

9. $\bar{1} \cdot 1/4,1/4,1/4$
   (9) $\bar{1} \cdot 1/2,1/2,1/2$

10. $n \cdot (1/2,1/2,0)$  
    (10) $n \cdot (1/2,1/2,0)$

11. $\bar{n} \cdot 0,0,0$  
    (11) $\bar{n} \cdot 0,0,0$

12. $\bar{n} \cdot 0,0,0$  
    (12) $\bar{n} \cdot 0,0,0$

13. $n' \cdot (1/2,0,1/2)$  
    (13) $n' \cdot (1/2,0,1/2)$

14. $n' \cdot 1/4,1/4,z$  
    (14) $n' \cdot 1/4,1/4,z$

15. $m' \cdot x,x,z$  
    (15) $m' \cdot x,x,z$

16. $m' \cdot x,x,z$  
    (16) $m' \cdot x,x,z$
Continued

### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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### Coordinates

| (1) | x,y,z [u,v,w]   |
| (2) | x,y,z [u,v,w]   |
| (3) | y+1/2,x+1/2,z+1/2 [v,u,w] |
| (4) | y+1/2,x+1/2,z+1/2 [v,u,w] |
| (5) | x,y,z [u,v,w]   |
| (6) | x,y,z [u,v,w]   |
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| (13) | x+1/2,y+1/2,z+1/2 [u,v,w] |
| (14) | x+1/2,y+1/2,z+1/2 [u,v,w] |
| (15) | y,x,z [u,v,w]   |
| (16) | y,x,z [u,v,w]   |
### Symmetry of Special Projections

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<th>Parameters</th>
<th>Origin</th>
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<td>Along ([0,0,1]) (p_1), 4mm</td>
<td>(a^* = (a - b)/2) (\quad b^* = (a + b)/2)</td>
<td>(1/2,0,0)</td>
</tr>
<tr>
<td>Along ([1,0,0]) (c2'mm')</td>
<td>(a^* = -c) (\quad b^* = b)</td>
<td>(x,0,0)</td>
</tr>
<tr>
<td>Along ([1,1,0]) (p2'mm')</td>
<td>(a^* = -c) (\quad b^* = (-a + b)/2)</td>
<td>(x,x,1/4)</td>
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### Details

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<td>([0,0,w])</td>
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<tr>
<td>2 (b)</td>
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<td>2''</td>
<td>([0,0,w])</td>
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<td>0,0,1/2</td>
<td>([0,0,w])</td>
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<tr>
<td>1/2,1,2,0</td>
<td>([0,0,w])</td>
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<td>([0,0,w])</td>
</tr>
<tr>
<td>2 (a)</td>
<td>4</td>
</tr>
<tr>
<td>2''</td>
<td>([0,0,w])</td>
</tr>
<tr>
<td>0,0,0</td>
<td>([0,0,w])</td>
</tr>
<tr>
<td>1/2,1,2,1/2</td>
<td>([0,0,w])</td>
</tr>
</tbody>
</table>
**Origin** at \(-\frac{1}{4},\frac{1}{4},\frac{1}{4}\) from center \((\overline{2/m'})\)

**Symmetry Operations**

1. \((1)\) 1
   \((1\mid 0,0,0)\)

2. \((2)\) \(2,0,0,z\)
   \((2\_z\mid 0,0,0)\)

3. \((3)\) \(4^{+}\) \((0,0,1/2)\) \(0,1/2,z\)
   \((4\_z\mid 1/2,1/2,1/2)\)

4. \((4)\) \(4^{-}\) \((0,0,1/2)\) \(1/2,0,z\)
   \((4\_z^{-}\mid 1/2,1/2,1/2)\)

5. \((5)\) \(2'\) \(0,y,0\)
   \((2\_y\mid 0,0,0)\)

6. \((6)\) \(2'\) \(x,0,0\)
   \((2\_x\mid 0,0,0)\)

7. \((7)\) \(2\) \((1/2,1/2,0)\) \(x,x,1/4\)
   \((2\_x\mid 1/2,1/2,1/2)\)

8. \((8)\) \(2\) \(x,x+1/2,1/4\)
   \((2\_x\mid 1/2,1/2,1/2)\)

9. \((9)\) \(\bar{1}\) \(1/4,1/4,1/4\)
   \((\bar{1}\mid 1/2,1/2,1/2)\)

10. \((10)\) \(n'\) \((1/2,1/2,0)\) \(x,y,1/4\)
    \((m\_y\mid 1/2,1/2,1/2)\)

11. \((11)\) \(\bar{4}^+\) \(0,0,z\) \(0,0,0\)
    \((\bar{4}\_z\mid 0,0,0)\)

12. \((12)\) \(\bar{4}^-\) \(0,0,0\) \(0,0,0\)
    \((\bar{4}\_z^{-}\mid 0,0,0)\)

13. \((13)\) \(n\) \((1/2,0,1/2)\) \(x,1/4,z\)
    \((m\_x\mid 1/2,1/2,1/2)\)

14. \((14)\) \(n\) \((0,1/2,1/2)\) \(1/4,y,z\)
    \((m\_y\mid 1/2,1/2,1/2)\)

15. \((15)\) \(m'\) \(x,x,z\)
    \((m\_x\mid 0,0,0)\)

16. \((16)\) \(m'\) \(x,x,z\)
    \((m\_x\mid 0,0,0)\)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>16</td>
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<tr>
<td>Generators</td>
<td>x,y,z</td>
<td>n+1/2,x+1/2,z+1/2</td>
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Continued

### Coordinates

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<tr>
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<td>x,y,z</td>
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<td>[u,v,w]</td>
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<tr>
<td>(3)</td>
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<td>[v,u,w]</td>
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<td>(4)</td>
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<td>[v,u,w]</td>
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<td>[u,v,w]</td>
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<td>(6)</td>
<td>x,y,z</td>
<td>[u,v,w]</td>
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<td>(7)</td>
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<td>[v,u,w]</td>
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<td>(12)</td>
<td>y,x,z</td>
<td>[v,u,w]</td>
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<td>(13)</td>
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<td>y,x,z</td>
<td>[v,u,w]</td>
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### Coordinates

<table>
<thead>
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<th>m</th>
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<tbody>
<tr>
<td>x,x,z</td>
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</tr>
<tr>
<td>x,x,z</td>
<td>[u,u,w]</td>
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<tr>
<td>x,x,z</td>
<td>[u,u,w]</td>
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<tr>
<td>x,x,z</td>
<td>[u,u,w]</td>
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### Coordinates

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<tr>
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### Coordinates

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<tbody>
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<tr>
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<td>[u,u,0]</td>
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<td>[u,u,0]</td>
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### Coordinates

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<tbody>
<tr>
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<td>[0,v,w]</td>
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</tr>
<tr>
<td>x,0,1/2</td>
<td>[0,v,w]</td>
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<td>[0,v,w]</td>
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### Coordinates

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<thead>
<tr>
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<tbody>
<tr>
<td>x,0,0</td>
<td>[0,v,w]</td>
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</tr>
<tr>
<td>x,0,0</td>
<td>[0,v,w]</td>
<td></td>
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<tr>
<td>x,0,0</td>
<td>[0,v,w]</td>
<td></td>
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<tr>
<td>x,0,0</td>
<td>[0,v,w]</td>
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### Coordinates

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<tbody>
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</tr>
<tr>
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### Coordinates

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<tr>
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<tr>
<td>0,0,z</td>
<td>[0,0,w]</td>
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<tr>
<td>0,0,z</td>
<td>[0,0,w]</td>
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### Coordinates

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<th>f</th>
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<tr>
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<tr>
<td>3/4,3/4,1/4</td>
<td>[0,0,0]</td>
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### Coordinates

<table>
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<th>e</th>
<th>..2/m'</th>
</tr>
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<tbody>
<tr>
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<tr>
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<td>[0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1/4,3/4,3/4</td>
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<td></td>
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### Coordinates

<table>
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<th>d</th>
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</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>0,1/2,1/4</td>
<td>[0,0,0]</td>
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<tr>
<td>0,1/2,1/4</td>
<td>[0,0,0]</td>
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<td>0,1/2,1/4</td>
<td>[0,0,0]</td>
<td></td>
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</tbody>
</table>
Continued

4 c 22'2'. 0,1/2,0 [0,0,w] 0,1/2,1/2 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,0 [0,0,w]
2 b 4'2'm' 0,0,1/2 [0,0,w] 1/2,1/2,0 [0,0,w]
2 a 4'2'm' 0,0,0 [0,0,w] 1/2,1/2,1/2 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p4'm'm
a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] c2mm1'
a* = b  b* = c
Origin at x,0,0

Along [1,1,0] p2m'm'
a* = (-a + b)/2  b* = c
Origin at x,x,1/4
Origin at \( \bar{4} \cdot 2/m' \) at \(-1/4, 1/4, -1/4\) from center \((2/m')\)

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq 1/2; & 0 \leq y & \leq 1; & 0 \leq z & \leq 1/4; & x & \leq y; & y & \leq 1-x
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) \quad 1 & \\
(2) \quad 2 & x,0,0 & (2_z,0,0) \\
(3) \quad 4 & (0,0,1/2) & 0,1/2,z & (4_z,1/2,1/2,1/2) \\
(4) \quad 4 & (0,0,1/2) & 1/2,0,z & (4_z,1/2,1/2,1/2) \\
(5) \quad 2 & 0,y,0 & (2_z,0,0) \\
(6) \quad 2 & x,0,0 & (2_z,0,0) \\
(7) \quad 2 & (1/2,1/2,0) & x,x,1/4 & (2_y,1/2,1/2,1/2) \\
(8) \quad 2 & x,y+1/2,1/4 & (2_y,1/2,1/2,1/2) \\
(9) \quad \bar{1} & 1/4,1/4,1/4 & (1,2,1/2,1/2) \\
(10) \quad n' & (1/2,1/2,0) & x,y,1/4 & (m_z,1/2,1/2,1/2)' \\
(11) \quad 4^{+} & 0,0,0 & 0,0,0 & (4_z,0,0,0)' \\
(12) \quad 4^{+} & 0,0,0 & 0,0,0 & (4_z,0,0,0)' \\
(13) \quad n' & (1/2,0,1/2) & x,1/4,z & (m_y,1/2,1/2,1/2)' \\
(14) \quad n' & (0,1/2,1/2) & 1/4,y,z & (m_y,1/2,1/2,1/2)' \\
(15) \quad m' & x,x,z & (m_y,0,0,0)' \\
(16) \quad m' & x,x,z & (m_y,0,0,0)' 
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>16 n 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w] (4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w] (6) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(7) y+1/2,x+1/2,z+1/2 [v,u,w] (8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<tr>
<td></td>
<td>(9) x+1/2,y+1/2,z+1/2 [u,v,w] (10) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<tr>
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<td>(11) y,x,z [v,u,w] (12) y,x,z [v,u,w]</td>
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<tr>
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<td>(13) x+1/2,y+1/2,z+1/2 [u,v,w] (14) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(15) y,x,z [v,u,w] (16) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>8 m ..m'</td>
<td>x,x,z [u,u,w] x,x,z [u,u,w] x+1/2,x+1/2,z+1/2 [u,u,w] x+1/2,x+1/2,z+1/2 [u,u,w]</td>
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<td>0,1/2,z [0,0,0] 0,1/2,z [0,0,0] 1/2,0,z+1/2 [1/2,0,0] 1/2,0,z+1/2 [1/2,0,0]</td>
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<tr>
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<td>0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0] 0,0,z [0,0,0] 1/2,1/2,z+1/2 [0,0,0]</td>
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<tr>
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<td>1/4,1/4,1/4 [0,0,0] 3/4,3/4,3/4 [0,0,0] 1/4,3/4,3/4 [0,0,0] 3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 d 2.22</td>
<td>0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 1/2,0,1/4 [0,0,0] 1/2,0,1/4 [0,0,0]</td>
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<td></td>
<td>0,1/2,1/4 [0,0,0] 0,1/2,1/4 [0,0,0] 1/2,0,1/4 [0,0,0] 1/2,0,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>( [0,0,1] )</td>
<td>p4m'</td>
<td>( 0,0,0 )</td>
</tr>
<tr>
<td>Symmetry</td>
<td>( a^* = \frac{a - b}{2} )</td>
<td>( b^* = \frac{a + b}{2} )</td>
</tr>
<tr>
<td>Origin</td>
<td>at ( 0,0,z )</td>
<td></td>
</tr>
<tr>
<td>( [1,0,0] )</td>
<td>c2m'</td>
<td>( x,0,0 )</td>
</tr>
<tr>
<td>Symmetry</td>
<td>( a^* = b )</td>
<td>( b^* = c )</td>
</tr>
<tr>
<td>Origin</td>
<td>at ( x,0,0 )</td>
<td></td>
</tr>
<tr>
<td>( [1,1,0] )</td>
<td>p2m'</td>
<td>( x,x,\frac{1}{4} )</td>
</tr>
<tr>
<td>Symmetry</td>
<td>( a^* = \frac{-a + b}{2} )</td>
<td>( b^* = c )</td>
</tr>
<tr>
<td>Origin</td>
<td>at ( x,x,\frac{1}{4} )</td>
<td></td>
</tr>
</tbody>
</table>
Origin at $\overline{4}2m$ at $-1/4,1/-4,-1/4$ from center (2/m)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/4; \quad x \leq y; \quad y \leq 1-x$

Symmetry Operations

For $(0,0,0) +$ set

(1) $1$
(1) $0,0,0$

(2) $2 \quad 0,0,z$
(2) $0,0,z$

(3) $4^* \quad (0,0,1/2) \quad 0,1/2,z$
(4) $2 \quad (0,1/2,1/2) \quad 1/2,0,z$

(4) $4^* \quad (0,0,1/2) \quad 1/2,0,z$
(4) $4^* \quad (0,1/2,1/2) \quad 1/2,0,z$

(5) $2 \quad 0,y,0$
(2) $0,y,0$

(6) $2 \quad x,0,0$
(2) $x,0,0$

(7) $2 \quad (1/2,1/2,0) \quad x,x,1/4$
(8) $2 \quad (1/2,1/2,0) \quad x,x,1/4$

(11) $m \quad x,x,z$
(11) $m \quad 1/2,1/2,1/2 +$ (1/2,1/2,1/2)

(12) $4 \quad 0,0,z; \quad 0,0,0$
(12) $4 \quad 0,0,z; \quad 0,0,0$

(9) $\overline{T} \quad 1/4,1/4,1/4$
(1) $1/2,1/2,1/2$

(10) $n \quad (1/2,1/2,0) \quad x,y,1/4$
(10) $n \quad (1/2,1/2,0) \quad x,y,1/4$

(11) $4^* \quad 0,0,z; \quad 0,0,0$
(11) $4^* \quad 0,0,z; \quad 0,0,0$

(13) $n \quad (1/2,0,1/2) \quad x,1/4,z$
(1) $1/2,1/2,1/2$

(14) $n \quad (0,1/2,1/2) \quad 1/4,y,z$
(14) $n \quad (0,1/2,1/2) \quad 1/4,y,z$

For $(1,0,0)' +$ set

(1) $t'(1,0,0)$
(1) $1,0,0$'

(2) $2' \quad 1/2,0,z$
(2) $1,0,0$'

(3) $4' \quad (0,0,1/2) \quad -1/2,0,z$
(4) $4' \quad (0,1/2,1/2) \quad -1/2,0,z$

(4) $4' \quad (0,0,1/2) \quad 1/2,0,z$
(4) $4' \quad (0,1/2,1/2) \quad 1/2,0,z$

(5) $2' \quad 1/2,y,0$
(2') $1,0,0$'

(6) $2' \quad (1,0,0) \quad x,0,0$
(2') $1,0,0$'

(7) $2' \quad (1/2,1/2,0) \quad x,x,1/4$
(8) $2' \quad (1/2,1/2,0) \quad x,x,1/4$

(9) $\overline{T} \quad 3/4,1/4,1/4$
(1) $3/2,1/2,1/2$

(10) $n' \quad (3/2,1/2,0) \quad x,y,1/4$
(10) $n' \quad (3/2,1/2,0) \quad x,y,1/4$

(11) $4^* \quad 1/2,-1/2,z; \quad 1/2,-1/2,0$
(11) $4^* \quad 1/2,-1/2,z; \quad 1/2,-1/2,0$

(12) $4^* \quad 1/2,1/2,1/2'$
(12) $4^* \quad 1/2,1/2,1/2'$

(13) $n' \quad (3/2,0,1/2) \quad x,1/4,z$
(1) $3/2,1/2,1/2$

(14) $n' \quad (0,1/2,1/2) \quad 3/4,y,z$
(14) $n' \quad (0,1/2,1/2) \quad 3/4,y,z$

Generators selected (1); $t'(1,0,0)$; $t'(0,1,0)$; $t'(0,0,1)$; (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 n 1</td>
<td>(0,0,0) + (1,0,0)' +</td>
</tr>
</tbody>
</table>

(1) $x,y,z \quad [u,v,w]$
(2) $x',y,z \quad [u',v',w]$
(3) $y+1/2,x+1/2,z+1/2 \quad [v,u,w]$
(4) $y+1/2,x+1/2,z+1/2 \quad [v,u,w]$
(5) $x,y,z \quad [u,v,w]$
(6) $x,y,z \quad [u,v,w]$
(7) $y+1/2,x+1/2,z+1/2 \quad [v,u,w]$
(8) $y+1/2,x+1/2,z+1/2 \quad [v,u,w]$
(9) $x+1/2,y+1/2,z+1/2 \quad [u,v,w]$
(10) $x+1/2,y+1/2,z+1/2 \quad [u,v,w]$
(11) $y,x,z \quad [v,u,w]$
(12) $y,x,z \quad [v,u,w]$
(13) $x+1/2,y+1/2,z+1/2 \quad [u,v,w]$
(14) $x+1/2,y+1/2,z+1/2 \quad [u,v,w]$

134.10.1141 - 2 - 2390
Continued

(15) \( \overline{y}, x, z \) \([v,u,w]\)

\(16 \ m \ .m \ x, x, z [u, u, 0] \)
\( \overline{x}, \overline{x}, z [u, u, 0] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, 0] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, 0] \)

(16) \( y, x, z \) \([\overline{v}, u, w]\)

\(16 \ l \ .2 \ x + 1/2, 3/4 [u, u, 0] \)
\( \overline{x}, \overline{x} + 1/2, 3/4 [u, u, 0] \)
\( x + 1/2, x, 3/4 [u, u, 0] \)
\( x + 1/2, x, 3/4 [u, u, 0] \)

Symmetry of Special Projections

Along [0,0,1] \( p4mm1' \)
\( a^* = (a - b)/2 \quad b^* = (a + b)/2 \)
Origin at 0,0,z

Along [1,0,0] \( c2mm1' \)
\( a^* = b \quad b^* = c \)
Origin at x,0,0

Along [1,1,0] \( p2mm1' \)
\( a^* = (a + b)/2 \quad b^* = c \)
Origin at x,x,1/4

134.10.1141 - P, 4_2/nmm
134.11.1142

$P_1 4_2 /n'n'm'$

4/mmm$1'$

Tetragonal

134.11.1142

$P_1 4_2 /n'2'n'2'm'$
Origin at $\bar{4}2'm'$ at -1/4,1/4,-1/4 from center ($2'm'$)

Asymmetric unit $0 \leq x \leq 1/2$; $0 \leq y \leq 1$; $0 \leq z \leq 1/4$; $x \leq y$; $y \leq 1-x$

Symmetry Operations

<table>
<thead>
<tr>
<th>Symmetry Operations</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1 (1</td>
<td>0,0,0)</td>
</tr>
<tr>
<td>(5) 2' x,0,0 (2z</td>
<td>0,0,0')</td>
</tr>
<tr>
<td>(9) $\bar{1}$/4,1/4,1/4 (1</td>
<td>1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(13) n' (1/2,0,1/2) x,1/4,z (m</td>
<td>1/2,1/2,1/2)'</td>
</tr>
</tbody>
</table>

For (1,0,0)' + set

| (1) t'(1,0,0) (1 | 0,0,0) | (2) 2' 1/2,0,z (2z | 1,0,0) | (3) 4' - (0,0,1/2) -1/2,2/0,z (4 | 3/2,1/2,1/2) | (4) 4' - (0,0,1/2) 0,1/2,z (4$z$ + 3/2,1/2,1/2) |
| (5) 2' 1/2,0,0 (2 | 0,0,0) | (6) 2' (1,0,0) x,0,0 (2z | 1,0,0) | (7) 2' x-1/2,x,1/4 (2 | 3/2,1/2,1/2) | (8) 2' (1/2,-1/2,0) x,$\bar{x}$+1/2,1/4 (2$\bar{x}$ | 3/2,1/2,1/2) |
| (9) $\bar{1}$/3,4,1/4,1/4 (1 | 3/2,1/2,1/2) | (10) n' (3/2,1/2,0) x,y,1/4 (m | 3/2,1/2,1/2) | (11) 4' - 1/2,-1/2,z; 1/2,-1/2,0 (4z | 1,0,0)' | (12) 4' - 1/2,1/2,z; 1/2,1/2,0 (4$z$ - 1,0,0) |
| (13) n (3/2,0,1/2) x,1/4,z (m | 3/2,1/2,1/2) | (14) n (0,1/2,1/2) 3/4,y,z (m | 3/2,1/2,1/2) | (15) g (1/2,-1/2,0) x+1/2,$\bar{x}$,z (m | 1,0,0) | (16) g (1/2,1/2,0) x+1/2,$\bar{x}$,z (m | 1,0,0) |

Generators selected

(1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>n 1</td>
<td>(0,0,0) + (1,0,0)' + (1,0,0), (0,0,1)', (0,1,0), (1,0,0)'</td>
</tr>
</tbody>
</table>

32

(1) x,y,z [u,v,w] (2) $\bar{x}$,$\bar{y}$,$\bar{z}$ [u,$\bar{v}$,$\bar{w}$] (3) $\bar{y}$+1/2,x+1/2,z+1/2 [v,$\bar{u}$,$\bar{w}$] (4) y+1/2,$\bar{x}$+1/2,z+1/2 [v,u,$w$] (5) $\bar{x}$,$\bar{y}$,$\bar{z}$ [u,$\bar{v}$,$\bar{w}$] (6) x,$\bar{y}$,$\bar{z}$ [u,v,w] (7) y+1/2,x+1/2,z+1/2 [v,$\bar{u}$,$\bar{w}$] (8) $\bar{y}$+1/2,$\bar{x}$+1/2,z+1/2 [v,u,$w$] (9) $\bar{x}$+1/2,$\bar{y}$+1/2,z+1/2 [u,v,w] (10) x+1/2,y+1/2,z+1/2 [u,$\bar{v}$,$\bar{w}$] (11) y,x,z [v,u,w] (12) $\bar{y}$,x,z [v,$\bar{u}$,$\bar{w}$] (13) x+1/2,$\bar{y}$+1/2,z+1/2 [u,$\bar{v}$,$\bar{w}$] (14) $\bar{x}$+1/2,y+1/2,z+1/2 [u,$\bar{v}$,$\bar{w}$]
Continued

(15) \( y, x, z [v, u, w] \)

(16) \( y, x, z [v, u, w] \)

16  m .m'
\( x, x, z [u, u, w] \)
---
\( x, x, z [u, u, w] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, w] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, w] \)

16  l .2'
\( x, x + 1/2, 3/4 [u, u, w] \)
---
\( x, x + 1/2, 1/4 [u, u, w] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, w] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, w] \)

16  k .2
\( x, x + 1/2, 1/4 [u, u, w] \)
---
\( x, x + 1/2, 1/4 [u, u, w] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, w] \)
\( x + 1/2, x + 1/2, z + 1/2 [u, u, w] \)

16  j .2,
\( x, 0, 1/2 [u, 0, 0] \)
---
\( x, 0, 1/2 [u, 0, 0] \)
\( x + 1/2, 1/2, 0 [u, 0, 0] \)
\( 0, x + 1/2, [0, 0, 0] \)

16  i .2',
\( x, 0, 1/2 [u, 0, 0] \)
---
\( x, 0, 1/2 [u, 0, 0] \)
\( x + 1/2, 1/2, 0 [u, 0, 0] \)
\( 0, x, 1/2 [0, 0, 0] \)

16  h .2',
\( x, 0, 1/2 [u, u, w] \)
---
\( x, 0, 1/2 [u, u, w] \)
\( x + 1/2, x + 1/2, 1/2 [u, u, w] \)
\( x + 1/2, x + 1/2, 1/2 [u, u, w] \)

8   g 2.m'm'
\( 0, 0, z [0, 0, w] \)
---
\( 0, 0, z [0, 0, w] \)
\( 0, 0, z [0, 0, w] \)
\( 0, 0, z [0, 0, w] \)

8   f .2/m'
\( 3/4, 3/4, 3/4 [0, 0, 0] \)
---
\( 1/4, 1/4, 3/4 [0, 0, 0] \)
\( 3/4, 1/4, 1/4 [0, 0, 0] \)
\( 1/4, 3/4, 1/4 [0, 0, 0] \)

8   e .2/m'
\( 1/4, 1/4, 1/4 [u, u, w] \)
---
\( 1/4, 3/4, 3/4 [u, u, w] \)
\( 3/4, 1/4, 3/4 [u, u, w] \)
\( 3/4, 1/4, 3/4 [u, u, w] \)

8   d .2',
\( 0, 1/2, 1/4 [u, u, w] \)
---
\( 0, 1/2, 1/4 [u, u, w] \)
\( 1/2, 0, 1/4 [u, u, w] \)
\( 1/2, 0, 1/4 [u, u, w] \)

8   c .2',
\( 0, 1/2, 0 [u, u, w] \)
---
\( 0, 1/2, 1/2 [0, 0, 0] \)
\( 1/2, 0, 1/2 [0, 0, 0] \)
\( 1/2, 0, 1/2 [0, 0, 0] \)

4   b \( \bar{4}2m' \)
\( 0, 0, 1/2 [0, 0, 0] \)
---
\( 0, 1/2, 0 [0, 0, 0] \)
\( 1/2, 1/2, 0 [0, 0, 0] \)
\( 1/2, 1/2, 0 [0, 0, 0] \)

4   a \( \bar{4}2m' \)
\( 0, 0, 0 [0, 0, w] \)
---
\( 0, 1/2, 0 [0, 0, 0] \)
\( 1/2, 1/2, 0 [0, 0, 0] \)
\( 1/2, 1/2, 0 [0, 0, 0] \)

Symmetry of Special Projections

Along [0,0,1] p4mm1'
\( a^* = (a - b)/2 \quad b^* = (a + b)/2 \)
Origin at 0,0,z

Along [1,0,0] c2mm1'
\( a^* = b \quad b^* = c \)
Origin at x,0,0

Along [1,1,0] p \( \bar{c} \) 2mm
\( a^* = -(a + b)/2 \quad b^* = c \)
Origin at x-1/4,x+1/4,1/4
Origin at center (2/m) at 42/m1n

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations:

1. $1$
2. $2 \cdot 0,0,z$
   \[ (2_z \cdot 0,0,0) \]
3. $4^+ (0,0,1/2) \cdot 0,0,z$
   \[ (4_z \cdot 0,0,1/2) \]
4. $4^- (0,0,1/2) \cdot 0,0,z$
   \[ (4_z^- \cdot 0,0,1/2) \]
5. $2 \cdot (0,1/2,0) \cdot 1/4,y,0$
   \[ (2_{z'} \cdot 1/2,1/2,0) \]
6. $2 \cdot (1/2,0,0) \cdot x,1/4,0$
   \[ (2_{z'} \cdot 1/2,1/2,0) \]
7. $2 \cdot (1/2,1,2,0) \cdot x,x,1/4$
   \[ (2_{y'} \cdot 1/2,1/2,1/2) \]
8. $2 \cdot x, x+1/2,1/4$
   \[ (2_{y'} \cdot 1/2,1/2,1/2) \]
9. $\bar{2} \cdot 0,0,0$
   \[ (\bar{2}_z \cdot 0,0,0) \]
10. $m \cdot x,y,0$
    \[ (m_z \cdot 0,0,0) \]
11. $4^+ \cdot 0,0,z; 0,0,1/4$
    \[ (4_z \cdot 0,0,1/2) \]
12. $4^- \cdot 0,0,z; 0,0,1/4$
    \[ (4_z^- \cdot 0,0,1/2) \]
13. $a \cdot (1/2,0,0) \cdot x,1/4,z$
    \[ (m_z \cdot 1/2,1/2,0) \]
14. $b \cdot (0,1/2,0) \cdot 1/4,y,z$
    \[ (m_z \cdot 1/2,1/2,0) \]
15. $c \cdot (0,0,1/2) \cdot x+1/2,\bar{x},z$
    \[ (m_{y'} \cdot 1/2,1/2,1/2) \]
16. $n \cdot (1/2,1/2,1/2) \cdot x,x,z$
    \[ (m_{y'} \cdot 1/2,1/2,1/2) \]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions
Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>i</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) x+1/2,y+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) x+1/2,y+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(7) x+1/2,y+1/2 [v,u,w]</td>
</tr>
<tr>
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<td>(9) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(11) y,x,z+1/2 [v,u,w]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(13) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(15) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>h</td>
<td>m..</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
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<td>y,x,1/2 [0,0,w]</td>
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<td>y+1/2,x+1/2,1/2 [0,0,w]</td>
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<tr>
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<td>g</td>
<td>..2</td>
<td>x,x+1/2,1/4 [u,u,0]</td>
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<td>x+1/2,x+1/2,3/4 [u,u,0]</td>
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<td>x+1/2,x+1/2,3/4 [u,u,0]</td>
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<tr>
<td>8</td>
<td>f</td>
<td>2..</td>
<td>0,1/2,z [0,0,w]</td>
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<td>0,1/2,z [0,0,w]</td>
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<td>0,1/2,z [0,0,w]</td>
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<td>0,1/2,z [0,0,w]</td>
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<td>0,1/2,1/4 [0,0,0]</td>
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<td>0,1/2,1/4 [0,0,0]</td>
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<td>0,1/2,1/4 [0,0,0]</td>
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<td></td>
<td></td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
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Symmetry of Special Projections

Along [0,0,1] p4gm1' a* = a  b* = b
Origin at 0,0,z

Along [1,0,0]  p222  2mm a* = b/2  b* = c
Origin at x,1/4,0

Along [1,1,0]  p222  2m'm' a* = -c/2  b* = (-a + b)/2
Origin at x,x,1/4

135.1.1143 - 2 - 2396
Origin at center (2/m1') at 4/m1n1'

Asymmetric unit

Asymmetric unit:
$$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$$

Symmetry Operations

For 1 + set

1. $1$
   (1) $0,0,0$

2. $2$
   (2) $0,0,z$
   (2) $0,0,0$

3. $4^+$
   (3) $(0,0,1/2)$
   (4) $(0,0,1/2)$

4. $4^-$
   (4) $(0,0,1/2)$
   (4) $(0,0,1/2)$

5. $2$
   (5) $(0,1/2,0)$
   (5) $(1/2,1/2,0)$

6. $2$
   (6) $(1/2,0,0)$
   (6) $(1/2,1/2,0)$

7. $2$
   (7) $(1/2,1/2,0)$
   (7) $(1/2,1/2,1/2)$

8. $2$
   (8) $(x,x+1/2,1/2)$
   (8) $(x,x+1/2,1/2)$

9. $2$
   (9) $0,0,0$
   (9) $0,0,0$

10. $m$
    (10) $x,y,0$
    (10) $x,y,0$

11. $4^+$
    (11) $0,0,1/4$
    (11) $0,0,1/4$

12. $4^-$
    (12) $0,0,1/4$
    (12) $0,0,1/4$

13. $a$
    (13) $(1/2,0,0)$
    (13) $(1/2,1/2,0)$

14. $b$
    (14) $(0,1/2,0)$
    (14) $(0,1/2,0)$

15. $c$
    (15) $(0,0,1/2)$
    (15) $(0,0,1/2)$

16. $n$
    (16) $(1/2,1/2,1/2)$
    (16) $(1/2,1/2,1/2)$
For 1' + set

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<tr>
<th>Generators selected</th>
<th>Coordinates</th>
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<tr>
<td>(1); t(0,0,0); t(0,1,0); t(1,0,0); (2); (3); (5); (9); 1'.</td>
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### Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>16</td>
<td>i</td>
<td>11'</td>
</tr>
</tbody>
</table>

| (1) | 1' | x,y,z [0,0,0] |
| (2) | 4' | x,y,z [0,0,0] |
| (3) | 2' | x,y,z [0,0,0] |
| (4) | 4' | x,y,z [0,0,0] |
| (5) | 2' | x,y,z [0,0,0] |
| (6) | 2' | x,y,z [0,0,0] |
| (7) | 2' | x,y,z [0,0,0] |
| (8) | 2' | x,y,z [0,0,0] |

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<th>m..1'</th>
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<td>x,y,z [0,0,0]</td>
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<td>(13)</td>
<td>2'</td>
<td>x,y,z [0,0,0]</td>
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<tr>
<td>(14)</td>
<td>2'</td>
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<tr>
<td>(15)</td>
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<td>x,y,z [0,0,0]</td>
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<td>(17)</td>
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<td>x,y,z [0,0,0]</td>
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<td>(23)</td>
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<td>(25)</td>
<td>2'</td>
<td>x,y,z [0,0,0]</td>
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<tr>
<td>(26)</td>
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<td>x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(28)</td>
<td>2'</td>
<td>x,y,z [0,0,0]</td>
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<tr>
<td>(29)</td>
<td>2'</td>
<td>x,y,z [0,0,0]</td>
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</table>

| 135.2.1144 - 2 - 2398 |
4  c  2/m..1'  0,1/2,0 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,0,0 [0,0,0]  0,1/2,1/2 [0,0,0]

4  b  4..1'  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]  1/2,1/2,3/4 [0,0,0]  1/2,1/2,1/4 [0,0,0]

4  a  2/m..1'  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p4gm1'</th>
<th>Along [1,0,0] p2mm1'</th>
<th>Along [1,1,0] p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a ) ( b^* = b )</td>
<td>( a^* = b/2 ) ( b^* = c )</td>
<td>( a^* = (-a + b)/2 ) ( b^* = c/2 )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,1/4</td>
</tr>
</tbody>
</table>
Origin at center (2/m') at $4_2/m'1n$

Asymmetric unit  
$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1  
(1 0,0,0)

(2) $2' \begin{pmatrix} 0,0,z \\ (2_z,0,0,0) \end{pmatrix}$

(3) $4' \begin{pmatrix} (0,0,1/2) \quad 0,0,z \\ (4_z,0,0,1/2) \end{pmatrix}$

(4) $4' \begin{pmatrix} (0,0,1/2) \quad 0,0,z \\ (4_z,0,0,1/2) \end{pmatrix}$

(5) $2' \begin{pmatrix} (0,1/2,0) \quad 1/4,y,0 \\ (2_y,1/2,1/2,0) \end{pmatrix}$

(6) $2' \begin{pmatrix} (1/2,0,0) \quad x,1/4,0 \\ (2_y,1/2,1/2,0) \end{pmatrix}$

(7) $2' \begin{pmatrix} (1/2,1/2,0) \quad x,x,1/4 \\ (2_y,1/2,1/2,1/2) \end{pmatrix}$

(8) $2' \begin{pmatrix} x,x+1/2,1/4 \\ (2_y,1/2,1/2,1/2) \end{pmatrix}$

(9) $\overline{1} \begin{pmatrix} 0,0,0 \\ (1,0,0,0) \end{pmatrix}$

(10) $m' \begin{pmatrix} x,y,0 \\ (m_z,0,0,0) \end{pmatrix}$

(11) $\overline{4} \begin{pmatrix} 0,0,z; 0,0,1/4 \\ (4_z,0,0,1/2) \end{pmatrix}$

(12) $\overline{4} \begin{pmatrix} 0,0,z; 0,0,1/4 \\ (4_z,0,0,1/2) \end{pmatrix}$

(13) $a \begin{pmatrix} (1/2,0,0) \quad x,1/4,z \\ (m_y,1/2,1/2,0) \end{pmatrix}$

(14) $b \begin{pmatrix} (0,1/2,0) \quad 1/4,y,z \\ (m_z,1/2,1/2,0) \end{pmatrix}$

(15) $c \begin{pmatrix} (0,0,1/2) \quad x+1/2,x,z \\ (m_y,1/2,1/2,1/2) \end{pmatrix}$

(16) $n \begin{pmatrix} (1/2,1/2,1/2) \quad x,x,z \\ (m_y,1/2,1/2,1/2) \end{pmatrix}$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions
Multiplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>16</td>
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<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<td></td>
<td></td>
<td>(3) x,y,z+1/2 [v,u,w]</td>
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<td>(4) y,x,z+1/2 [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td></td>
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<td>(6) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(7) y+1/2,x+1/2,z [u,v,w]</td>
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<td>(8) y+1/2,x,z+1/2 [v,u,w]</td>
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<td>(9) x+1/2,y,z [u,v,w]</td>
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<td>(10) x,y,z [u,v,w]</td>
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<td>(11) y,x,z+1/2 [v,u,w]</td>
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<td>(12) y,x,1/2 [v,u,w]</td>
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<td>(13) x+1/2,y,z+1/2 [u,v,w]</td>
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<td>(14) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(15) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<tr>
<td>8</td>
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<td>x,y,0 [u,v,0]</td>
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<tr>
<td></td>
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<td>x,y,0 [u,v,0]</td>
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<td>x,y+1/2,z [u,v,0]</td>
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<td>y,x+1/2 [v,u,0]</td>
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<td>y,x+1/2 [v,u,0]</td>
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<td>x+1/2,y+1/2,z [u,v,0]</td>
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<td>x,x+1/2,1/4 [u,u,w]</td>
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Symmetry of Special Projections
Along [0,0,1] p4gm  
Origin at 0,0,z  

Along [1,0,0] p2ar 2m'm'  
a* = b  
b* = c  
Origin at x,0,0

Along [1,1,0] p2ar 2m'm'  
a* = -c/2  
b* = (-a + b)/2  
Origin at x,x,0
Origin at center (2/m) at 42'/m1n

Asymmetric unit

\[0 < x < \frac{1}{2}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{4}\]

Symmetry Operations

1. \[1\]
   \[
   (1 \mid 0,0,0)
   \]
2. \[2\]
   \[
   0,0,z
   
   (2_z \mid 0,0,0)
   \]
3. \[4^+\]
   \[
   (0,0,1/2) \quad 0,0,z
   
   (4_z \mid 0,0,1/2)'
   \]
4. \[4^-\]
   \[
   (0,0,1/2) \quad 0,0,z
   
   (4_z \mid 0,0,1/2)'
   \]
5. \[2'\]
   \[
   (0,1/2,0) \quad 1/4,y,0
   
   (2_z \mid 1/2,1/2,0)'
   \]
6. \[2'\]
   \[
   (1/2,0,0) \quad x,1/4,0
   
   (2_z \mid 1/2,1/2,0)'
   \]
7. \[2\]
   \[
   (1/2,1/2,0) \quad x,x,1/4
   
   (2_{xy} \mid 1/2,1/2,1/2)
   \]
8. \[2\]
   \[
   x,x+1/2,1/4
   
   (2_{xy} \mid 1/2,1/2,1/2)
   \]
9. \[\bar{1}\]
   \[
   0,0,0
   
   (1 \mid 0,0,0)
   \]
10. \[m\]
    \[
    x,y,0
    
    (m_o \mid 0,0,0)
    \]
11. \[\bar{4}^+\]
    \[
    0,0,z
    
    (4_z \mid 0,0,1/2)'
    \]
12. \[\bar{4}^-\]
    \[
    0,0,z
    
    (4_z \mid 0,0,1/2)'
    \]
13. \[a'\]
    \[
    (1/2,0,0) \quad x,1/4,z
    
    (m_y \mid 1/2,1/2,0)'
    \]
14. \[b'\]
    \[
    (0,1/2,0) \quad 1/4,y,z
    
    (m_x \mid 1/2,1/2,0)'
    \]
15. \[c\]
    \[
    (0,0,1/2) \quad x+1/2,x,z
    
    (m_{xy} \mid 1/2,1/2,1/2)
    \]
16. \[n\]
    \[
    (1/2,1/2,1/2) \quad x,x,z
    
    (m_{xy} \mid 1/2,1/2,1/2)
    \]

---

135.4.1146 - 1 - 2402
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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### Coordinates

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### Symmetry of Special Projections

- **Along [0,0,1]**: p4gm1'
  - $a^* = a$
  - $b^* = b$
  - Origin at 0,0,z

- **Along [1,0,0]**: p2'2'm'
  - $a^* = -c$
  - $b^* = b/2$
  - Origin at x,0,0

- **Along [1,1,0]**: p2'2'm'
  - $a^* = -c/2$
  - $b^* = (-a + b)/2$
  - Origin at x,x,1/4
Origin at center (2/m) at 4/m1n'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \]

Symmetry Operations

1. 1
2. \[ 2 \; 0,0,z \] 
   \[ (z_1:0,0,0) \]
3. \[ 4^+ \cdot (0,0,1/2) \; 0,0,z \] 
   \[ (z_2:0,0,1/2') \]
4. \[ 4^- \cdot (0,0,1/2) \; 0,0,z \] 
   \[ (z_2:-1:0,0,1/2') \]
5. \[ 2 \; (0,1/2,0) \; 1/4,y,0 \] 
   \[ (z_1:1/2,1/2,0) \]
6. \[ 2 \; (1/2,0,0) \; x,1/4,0 \] 
   \[ (z_1:1/2,1/2,0) \]
7. \[ 2' \; (1/2,1/2,0) \; x,x,1/4 \] 
   \[ (z_{xy}:1/2,1/2,1/2') \]
8. \[ 2' \; x,x+1/2,1/4 \] 
   \[ (z_{xy}:1/2,1/2,1/2') \]
9. \[ \overline{1} \; 0,0,0 \] 
   \[ (1:0,0,0) \]
10. \[ m \; x,y,0 \] 
    \[ (m_1:0,0,0) \]
11. \[ 4^+ \cdot \; 0,0,z \; 0,0,1/4 \] 
    \[ (z_2:0,0,1/2') \]
12. \[ 4^- \cdot \; 0,0,z \; 0,0,1/4 \] 
    \[ (z_2:-1:0,0,1/2') \]
13. \[ a \; (1/2,0,0) \; x,1/4,z \] 
    \[ (m_3:1/2,1/2,0) \]
14. \[ b \; (0,1/2,0) \; 1/4,y,z \] 
    \[ (m_3:1/2,2,2,0) \]
15. \[ c' \; (0,0,1/2) \; x+1/2,\overline{z},z \] 
    \[ (m_{xy}:1/2,1/2,1/2') \]
16. \[ n' \; (1/2,1/2,1/2) \; x,x,z \] 
    \[ (m_{xy}:1/2,1/2,1/2') \]
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

**Generators**

- **(1)**: \(x, y, z\ [u, v, w]\)
- **(2)**: \(x, y, z\ [u, v, w]\)
- **(3)**: \(y, x, z + 1/2\ [v, u, w]\)
- **(4)**: \(y, x, z + 1/2\ [v, u, w]\)
- **(5)**: \(x + 1/2, y + 1/2, z\ [u, v, w]\)
- **(6)**: \(y + 1/2, x + 1/2, z + 1/2\ [v, u, w]\)
- **(7)**: \(y + 1/2, x + 1/2, z\ [u, v, w]\)
- **(8)**: \(y + 1/2, x + 1/2, z\ [u, v, w]\)
- **(9)**: \(x + 1/2, y + 1/2, z\ [u, v, w]\)
- **(10)**: \(x, y, z\ [u, v, w]\)
- **(11)**: \(y, x, z + 1/2\ [v, u, w]\)
- **(12)**: \(y, x, z + 1/2\ [v, u, w]\)
- **(13)**: \(y + 1/2, y + 1/2, z\ [u, v, w]\)
- **(14)**: \(y + 1/2, x + 1/2, z\ [u, v, w]\)
- **(15)**: \(y + 1/2, x + 1/2, z + 1/2\ [v, u, w]\)
- **(16)**: \(y + 1/2, x + 1/2, z + 1/2\ [v, u, w]\)

**Symmetry of Special Projections**

- **Along [0,0,1] p4gm1'**
  - **a = a**
  - **b' = b**
  - **Origin at 0,0,z**

- **Along [1,0,0] p2a 2mm**
  - **a' = b/2**
  - **b' = c**
  - **Origin at x,1/4,0**

- **Along [1,1,0] p2m'**
  - **a' = (-a + b)/2**
  - **b' = c/2**
  - **Origin at x,x,1/4**

---

135.5.1147 - 2 - 2405
**Origin** at center \((2/m')\) at \(4_2'/m'1n\)

**Asymmetric unit**

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4
\]

**Symmetry Operations**

\begin{align*}
(1) \, & (1 | 0,0,0) \\
(2) \, & \begin{pmatrix} 2 \quad 0,0,z \\ 2_z \quad 0,0,0 \end{pmatrix} \\
(3) \, & 4' \cdot (0,0,1/2) \quad 0,0,z \\
& \quad (4_z \quad 0,0,1/2') \\
(4) \, & 4' \cdot (0,0,1/2) \quad 0,0,z \\
& \quad (4_z \quad 0,0,1/2') \\
(5) \, & \begin{pmatrix} 2 \quad (0,1/2,0) \\ (2_z) \quad 1/2,1/2,0 \end{pmatrix} \\
(6) \, & \begin{pmatrix} 2 \quad (1/2,0,0) \\ (2_z) \quad 1/2,1/2,0 \end{pmatrix} \\
(9) \, & \begin{pmatrix} 1' \quad 0,0,0 \\ (1' \quad 0,0,0)' \end{pmatrix} \\
(10) \, & \begin{pmatrix} m' \quad x,y,0 \\ (m_z) \quad 0,0,0)' \end{pmatrix} \\
(11) \, & \begin{pmatrix} 4' \quad 0,0,z; 0,0,1/4 \\ (4_z) \quad 0,0,1/2 \end{pmatrix} \\
(12) \, & \begin{pmatrix} 4' \quad 0,0,z; 0,0,1/4 \\ (4_z') \quad 0,0,1/2 \end{pmatrix} \\
(13) \, & \begin{pmatrix} a' \quad (1/2,0,0) \\ (m_z) \quad 1/2,1/2,0)' \end{pmatrix} \\
(14) \, & \begin{pmatrix} b' \quad (0,1/2,0) \\ (m_z) \quad 1/2,1/2,0)' \end{pmatrix} \\
(15) \, & \begin{pmatrix} c \quad (0,0,1/2) \\ (m_{xy}) \quad 1/2,1/2,1/2 \end{pmatrix} \\
(16) \, & \begin{pmatrix} n \quad (1/2,1/2,1/2) \\ x,x,z \end{pmatrix}
\end{align*}
### Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</table>
| 16           | i              | 1 (1) x,y,z [u,v,w]  
|              |                | (2) x,y,z [u,v,w]  
|              |                | (3) y,x,z+1/2 [v,u,w]  
|              |                | (4) y,x,z+1/2 [v,u,w]  
|              |                | (5) x+1/2,y+1/2,z [u,v,w]  
|              |                | (6) y+1/2,x+1/2,z+1/2 [v,u,w]  
|              |                | (7) x+1/2,y+1/2,z [u,v,w]  
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|              |                | (10) x,y,z [u,v,w]  
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|              |                | (12) y,x,z+1/2 [v,u,w]  
|              |                | (13) y+1/2,x+1/2,z [u,v,w]  
|              |                | (14) y,x,z+1/2 [v,u,w]  
|              |                | (15) y+1/2,x+1/2,z+1/2 [v,u,w]  
|              |                | (16) y+1/2,x+1/2,z+1/2 [v,u,w]  
| 8            | h              | m'.. x,y,0 [u,v,0]  
|              |                | x,y,0 [u,v,0]  
|              |                | y,x,1/2 [v,u,0]  
|              |                | y,x,1/2 [v,u,0]  
|              |                | y+1/2,x+1/2,1/2 [v,u,0]  
|              |                | x+1/2,y+1/2,0 [v,u,0]  
| 8            | g              | ..2' x,x+1/2,1/4 [u,u,w]  
|              |                | x,x+1/2,1/4 [u,u,w]  
|              |                | x+1/2,x,3/4 [u,u,w]  
|              |                | x+1/2,x,1/4 [u,u,w]  
|              |                | x+1/2,x,1/4 [u,u,w]  
| 8            | f              | 2.. 0,1/2,z [0,0,w]  
|              |                | 0,1/2,z [0,0,w]  
|              |                | 0,1/2,z [0,0,w]  
|              |                | 0,1/2,z [0,0,w]  
| 8            | e              | 2.. 0,0,z [0,0,w]  
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|              |                | 0,0,z+1/2 [0,0,w]  
|              |                | 0,0,z+1/2 [0,0,w]  
|              |                | 0,0,z+1/2 [0,0,w]  
| 4            | d              | 2.2'2' 0,1/2,1/4 [0,0,w]  
|              |                | 0,1/2,1/4 [0,0,w]  
|              |                | 0,1/2,1/4 [0,0,w]  
|              |                | 0,1/2,1/4 [0,0,w]  
| 4            | c              | 2/m'.. 0,1/2,0 [0,0,0]  
|              |                | 1/2,0,0 [0,0,0]  
|              |                | 1/2,0,0 [0,0,0]  
|              |                | 1/2,0,0 [0,0,0]  
| 4            | b              | 4.. 0,0,1/4 [0,0,w]  
|              |                | 0,0,3/4 [0,0,w]  
|              |                | 0,0,3/4 [0,0,w]  
|              |                | 0,0,3/4 [0,0,w]  
| 4            | a              | 2/m'.. 0,0,0 [0,0,0]  
|              |                | 0,0,1/2 [0,0,0]  
|              |                | 0,0,1/2 [0,0,0]  
|              |                | 0,0,1/2 [0,0,0]  

### Symmetry of Special Projections

- **Along [0,0,1]**: p4'g'm
  - \( \mathbf{a}^* = \mathbf{a} \)
  - \( \mathbf{b}^* = \mathbf{b} \)
  - Origin at 0,0,z

- **Along [1,0,0]**: p2m'm'
  - \( \mathbf{a}^* = \mathbf{b}/2 \)
  - \( \mathbf{b}^* = \mathbf{c} \)
  - Origin at x,0,0

- **Along [1,1,0]**: \( p_{2x} \)
  - \( \mathbf{a}^* = -\mathbf{c}/2 \)
  - \( \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \)
  - Origin at x,x,0
Origin at center (2/m) at 4/m21'\slash b'2'/c'

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
(1 | 0,0,0)

(5) 2' (0,1/2,0) 1/4,y,0
(2,1/2,1/2,0')

(9) 0,0,0
(1 | 0,0,0)

(13) a' (1/2,0,0) x,1/4,z
(m,1/2,1/2,0')

(2) 2 0,0,z
(2z|0,0,0)

(6) 2' (1/2,0,0) x,1/4,0
(2z|1/2,1/2,0')

(10) m x,y,0
(m|0,0,0)

(14) b' (0,1/2,0) 1/4,y,z
(m,1/2,1/2,0')

(3) 4' (0,0,1/2) 0,0,z
(4z|0,0,1/2)

(7) 2' (1/2,1/2,0) x,x,1/4
(2xy|1/2,1/2,1/2')

(11) 4' 0,0,z; 0,0,1/4
(4z|0,0,1/2)

(15) c' (0,0,1/2) x+1/2,\bar{z},z
(m,1/2,1/2,1/2')

(4) 4' (0,0,1/2) 0,0,z
(4z|0,0,1/2)

(8) 2' x,x+1/2,1/4
(2xy|1/2,1/2,1/2')

(12) 4' 0,0,z; 0,0,1/4
(4z|0,0,1/2)

(16) n' (1/2,1/2,1/2) x,x,z
(m,1/2,1/2,1/2')
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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8 h m.. x,y,0 [0,0,w] x,y,0 [0,0,w] y,x,1/2 [0,0,w] y,x,1/2 [0,0,w] x+1/2,y+1/2,0 [0,0,w] x+1/2,y+1/2,0 [0,0,w] y+1/2,x+1/2,1/2 [0,0,w] y+1/2,x+1/2,1/2 [0,0,w]

8 g ..2' x,x+1/2,1/4 [u,u,w] x,x+1/2,1/4 [u,u,w] x+1/2,x,3/4 [u,u,w] x+1/2,x,3/4 [u,u,w] x+1/2,x,3/4 [u,u,w] x+1/2,x,3/4 [u,u,w] x+1/2,x,1/4 [u,u,w] x+1/2,x,1/4 [u,u,w]

8 f 2.. 0,1/2,z [0,0,w] 0,1/2,z [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w] 1/2,0,z+1/2 [0,0,w]

8 e 2.. 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w] 1/2,1/2,z [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w] 1/2,1/2,z+1/2 [0,0,w]

4 d 2.2'2' 0,1/2,1/4 [0,0,w] 0,1/2,1/4 [0,0,w] 1/2,0,3/4 [0,0,w] 1/2,0,3/4 [0,0,w] 0,1/2,3/4 [0,0,w] 0,1/2,3/4 [0,0,w] 0,1/2,3/4 [0,0,w] 0,1/2,3/4 [0,0,w]

4 c 2/m.. 0,1/2,0 [0,0,w] 0,1/2,0 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w] 1/2,0,1/2 [0,0,w]

4 b 4.. 0,0,1/4 [0,0,w] 0,0,3/4 [0,0,w] 1/2,1/2,3/4 [0,0,w] 1/2,1/2,3/4 [0,0,w] 1/2,1/2,3/4 [0,0,w] 1/2,1/2,3/4 [0,0,w] 1/2,1/2,3/4 [0,0,w] 1/2,1/2,3/4 [0,0,w]

4 a 2/m.. 0,0,0 [0,0,w] 0,0,1/2 [0,0,w] 1/2,1/2,0 [0,0,w] 1/2,1/2,0 [0,0,w] 1/2,1/2,0 [0,0,w] 1/2,1/2,0 [0,0,w] 1/2,1/2,0 [0,0,w] 1/2,1/2,0 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p4gm1’

a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p2mm’

a* = -c  b* = b/2
Origin at x,0,0

Along [1,1,0] p2m’m’

a* = -(a + b)/2  b* = c/2
Origin at x,x,1/4
Origin at center (2/m') at 4_2/m'1m'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
(1) 0,0,0

(5) 2' (0,1/2,0) 1/4,y,0
(2_z) 1/2,1/2,0,

(9) 11' 0,0,0
(1) 0,0,0,

(13) a (1/2,0,0) x,1/4,z
(m_y) 1/2,1/2,0,

(1) 0,0,0

(2) 2 0,0,z
(2_z) 0,0,0

(6) 2' (1/2,0,0) x,1/4,0
(2_z) 1/2,1/2,0,

(10) m' x,y,0
(m_z) 0,0,0,

(11) 4+ * (0,0,1/2) 0,0,z
(4_z) 0,0,1/2

(14) b (0,1/2,0) 1/4,y,z
(m_y) 1/2,1/2,0,

(3) 4+ * (0,0,1/2) 0,0,z
(4_z) 0,0,1/2

(7) 2 (1/2,1/2,0) x,x,1/4
(2_y) 1/2,1/2,1/2

(15) c' (0,0,1/2) x+1/2,x,z
(m_y) 1/2,1/2,1/2,

(4) 4+ * (0,0,1/2) 0,0,z
(4_z) 0,0,1/2

(8) 2 x,x+1/2,1/4
(2_y) 1/2,1/2,1/2

(12) 4+ * 0,0,z; 0,0,1/4
(4_z) 0,0,1/2

(13) a (1/2,0,0) x,1/4,z
(m_y) 1/2,1/2,0,

(16) n' (1/2,1/2,1/2) x,x,z
(m_y) 1/2,1/2,1/2,

(14) b (0,1/2,0) 1/4,y,z
(m_y) 1/2,1/2,0,
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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<th>Coordinates</th>
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Symmetry of Special Projections

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<th>Origin</th>
<th>[0,0,1]</th>
<th>4p4'gm'</th>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
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<td>a* = a</td>
<td>b* = b</td>
<td></td>
<td>a* = b/2</td>
<td>b* = c</td>
<td>a* = (a + b)/2</td>
<td>b* = c/2</td>
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<td>Origin at 0,0,z</td>
<td>Along [1,0,0]</td>
<td>p2m'm'</td>
<td>Along [1,1,0]</td>
<td>p2m'm'</td>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

135.8.1150 - 2 - 2411
Origin at center (2/m') at 4/m'm'1n'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4

Symmetry Operations

(1) 1
    (1|0,0,0)
(5) 2 (0,1/2,0) 1/4,y,0
    (2,1/2,1/2,0)
(9) 1' 0,0,0
    (1|0,0,0)
(13) a' (1/2,0,0) x,1/4,z
    (m,1/2,1/2,0)
(2) 2 0,0,z
    (2,0,0,0)
(6) 2 (1/2,0,0) x,1/4,0
    (2,1/2,1/2,0)
(10) m' x,y,0
    (m,0,0,0)
(14) b' (0,1/2,0) 1/4,y,z
    (m,1/2,1/2,0)
(3) 4' (0,0,1/2) 0,0,z
    (4,0,0,1/2)
(7) 2 (1/2,1/2,0) x,x,1/4
    (2,1/2,1/2,1/2)
(11) 4' 0,0,z
    (4,0,0,1/2)
(8) 2 x,x+1/2,1/4
    (2,2,1/2,1/2)
(12) 4' 0,0,z
    (4,0,0,1/2)
(15) c' (0,0,1/2) x+1/2,x,z
    (m,1/2,1/2,1/2)
(16) n' (1/2,1/2,1/2) x,x,z
    (m,1/2,1/2,1/2)

P4₁/m'b'c'
135.9.1151

4/m'm'm'

P4₁/m'2₁/b'2/c'

Tetragonal
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<th>Site Symmetry</th>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>4</td>
<td>a</td>
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<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4g'm'
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p 2m'm'
\( a^* = b/2 \quad b^* = c \)
Origin at x,0,0

Along [1,1,0] p2m'm'
\( a^* = (-a + b)/2 \quad b^* = c/2 \)
Origin at x,x,0

135.9.1151 - 2 - 2413
Origin at center (mmm) at 2/m12/m

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

Symmetry Operations

(1) 1
(1|0,0,0)

(5) 2 (0,1/2,0) 1/4,y,1/4
(2|1/2,1/2,1/2)

(9) \(\overline{1}\) 0,0,0
(1|0,0,0)

(13) n (1/2,0,1/2) x,1/4,z
(0|1/2,1/2,1/2)

(2) 2 0,0,z
(2z|0,0,0)

(6) 2 (1/2,0,0) x,1/4,1/4
(2z|1/2,1/2,1/2)

(10) m x,y,0
(m|0,0,0)

(14) n (0,1/2,1/2) 1/4,y,z
(m|1/2,1/2,1/2)

(3) 4^+ (0,0,1/2) 0,1/2,z
(4z|1/2,1/2,1/2)

(7) 2 x,x,0
(2xy|0,0,0)

(11) 4^- 1/2,0,z; 1/2,0,1/4
(4z^-|1/2,1/2,1/2)

(15) m x,x,z
(mxy|0,0,0)

(4) 4^- (0,0,1/2) 1/2,0,z
(4z^-|1/2,1/2,1/2)

(8) 2 x,x,0
(2xy|0,0,0)

(12) 4^- 0,1/2,z; 0,1/2,1/4
(4z^-|1/2,1/2,1/2)

(16) m x,x,z
(mxy|0,0,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>16 k 1</td>
<td>(1) (x,y,z \ [u,v,w])</td>
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<tr>
<td></td>
<td>(3) (y+1/2,x+1/2,z+1/2 \ [v,u,w])</td>
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<td>(5) (x+1/2,y+1/2,z+1/2 \ [u,v,w])</td>
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<td>(15) (y,x,z \ [v,u,w])</td>
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<tr>
<td>8 j ..m</td>
<td>(x,x,z \ [u,u,0])</td>
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<td>(x+1/2,x+1/2,z+1/2 \ [u,u,0])</td>
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<td>(x+1/2,x+1/2,z+1/2 \ [u,u,0])</td>
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<td>8 i m..</td>
<td>(x,y,0 \ [0,0,w])</td>
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<td>(y+1/2,x+1/2,1/2 \ [0,0,w])</td>
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<td>(x+1/2,y+1/2,1/2 \ [0,0,w])</td>
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<td>8 h 2..</td>
<td>(0,1/2,z \ [0,0,w])</td>
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<td>(1/2,0,z+1/2 \ [0,0,w])</td>
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<tr>
<td>4 g m.2m</td>
<td>(x,\bar{x},0 \ [0,0,0])</td>
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<td>(\bar{x},x,0 \ [0,0,0])</td>
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<td>4 e 2.mm</td>
<td>(0,0,z \ [0,0,0])</td>
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<td>(1/2,1/2,z+1/2 \ [0,0,0])</td>
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<td>(1/2,0,1/2 \ [0,0,w])</td>
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<tr>
<td>2 b m.mm</td>
<td>(0,0,1/2 \ [0,0,0])</td>
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</tbody>
</table>
Continued

2 a m.mm 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4gm1’
\[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,1/2,z

Along [1,0,0] c_p 2’mm’
\[ \mathbf{a}^* = -\mathbf{c}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at x,0,0

Along [1,1,0] p2mm1’
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2, \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,0
**Origin** at center (mmm1\' ) at 2/m12/m1'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq y \]

**Symmetry Operations**

\[ 1 + \text{set} \]

1. \( 1 \) \[ (1 | 0,0,0) \]
2. \( 2 \) \[ (0,0,z) \]
3. \( 4^+ (0,0,1/2) \) \[ 0,1/2,z \]
4. \( 4^- (0,0,1/2) \) \[ 1/2,0,z \]
5. \( 2 \) \[ (0.1/2,0) \] \[ 1/4,y,z \]
6. \( 2 \) \[ (1/2,0,0) \] \[ 1/4,y,z \]
7. \( 2 \) \[ x,x,0 \]
8. \( 2 \) \[ x,x,0 \]
9. \( \bar{1} \) \[ 0,0,0 \]
10. \( m \) \[ x,y,0 \]
11. \( 4^+ 1/2,0,z \) \[ 1/2,1/2,1/2 \]
12. \( 4^- 0,1/2,z \) \[ 0,1/2,1/2 \]
13. \( n \) \[ (1/2,0,1/2) \] \[ x,1/4,z \]
14. \( n \) \[ (0,1/2,1/2) \] \[ 1/4,y,z \]
15. \( m \) \[ x,x,z \]
16. \( m \) \[ x,x,z \]
Continued

$P4_{2}/mnm1'$

1' + set

(1) 1' (1) 0,0,0')
(2) 2' 0,0,z (2) 0,0,0')
(3) 4' (0,0,1/2) 0,1/2,z (4) 4' (0,0,1/2) 1/2,0,z
(5) 2' (0,1/2,0) 1/4,y,1/4 (6) 2' (1/2,0,0) x,1/4,1/4
(7) 2' x,x,0 (8) 2' x,x,0
(9) 1' 0,0,0' (10) m' x,y,0 (11) 4' 1/2,0,z; 1/2,0,1/4
(12) 4' 0,1/2,z; 0,1/2,1/4
(13) n' (1/2,0,1/2) x,1/4,z (14) n' (0,1/2,1/2) 1/4,y,z
(15) m' x,x,z (16) m' x,x,z

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

Positions

Multiplicity
Wyckoff letter
Site Symmetry.

1 + 1' +

16  k  11'

(1) x,y,z [0,0,0]
(2) x,y,z [0,0,0]
(3) y+1/2,x+1/2,z+1/2 [0,0,0]
(4) y+1/2,x+1/2,z+1/2 [0,0,0]
(5) x+1/2,y+1/2,z+1/2 [0,0,0]
(6) x+1/2,y+1/2,z+1/2 [0,0,0]
(7) y,x,z [0,0,0]
(8) y,x,z [0,0,0]
(9) x,y,z [0,0,0]
(10) x,y,z [0,0,0]
(11) y+1/2,x+1/2,z+1/2 [0,0,0]
(12) y+1/2,x+1/2,z+1/2 [0,0,0]
(13) x+1/2,y+1/2,z+1/2 [0,0,0]
(14) x+1/2,y+1/2,z+1/2 [0,0,0]
(15) y,x,z [0,0,0]
(16) y,x,z [0,0,0]

8  j .m1'

x,x,z [0,0,0] x,x,z [0,0,0]
(2) x,y,z [0,0,0]
(4) y+1/2,x+1/2,z+1/2 [0,0,0]
(6) x+1/2,y+1/2,z+1/2 [0,0,0]
(9) x,x,z [0,0,0]
(11) y+1/2,x+1/2,z+1/2 [0,0,0]
(13) x+1/2,y+1/2,z+1/2 [0,0,0]
(15) y,x,z [0,0,0]

8  i m..1'

x,y,0 [0,0,0] x,y,0 [0,0,0]
(2) x,y,0 [0,0,0]
(4) y+1/2,x+1/2,1/2 [0,0,0]
(6) x+1/2,y+1/2,1/2 [0,0,0]
(9) x,x,0 [0,0,0]
(11) y+1/2,x+1/2,1/2 [0,0,0]
(13) x+1/2,y+1/2,1/2 [0,0,0]
(15) y,x,0 [0,0,0]
| 8  | h  | 2..1' | 0,1/2,z [0,0,0] | 0,1/2,z+1/2 [0,0,0] | 1/2,0, z+1/2 [0,0,0] | 1/2,0, z [0,0,0] |
| 4  | g  | m.2m1' | x,x,0 [0,0,0] | x+1/2,x+1/2,1/2 [0,0,0] | x+1/2,x,1/2,1/2 [0,0,0] |
| 4  | f  | m.2m1' | x,x,0 [0,0,0] | x+1/2,x+1/2,1/2 [0,0,0] | x+1/2,x,1/2,1/2 [0,0,0] |
| 4  | e  | 2.mm1' | 0,0,z [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] | 1/2,1/2,z+1/2 [0,0,0] |
| 4  | d  | 4'..1' | 0,1/2,1/4 [0,0,0] | 1/2,0,1/4 [0,0,0] | 1/2,0,3/4 [0,0,0] |
| 4  | c  | 2/m..1' | 0,1/2,0 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,0,0 [0,0,0] |
| 2  | b  | m.mm1' | 0,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 2  | a  | m.mm1' | 0,0,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

**Symmetry of Special Projections**

- **Along [0,0,1] p4gm1'**
  - \( a^* = a \quad b^* = b \)
  - Origin at 0,1/2,z

- **Along [1,0,0] c2mm1'**
  - \( a^* = b \quad b^* = c \)
  - Origin at x,0,0

- **Along [1,1,0] p2mm1'**
  - \( a^* = (-a + b)/2 \quad b^* = c \)
  - Origin at x,x,0
Origin at center (mmm') at 2/m'12'/m

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

(1) 1  
(1) 0,0,0

(2) 2 0,0,z  
(2) 0,0,0

(3) 4' (0,0,1/2) 0,1/2,z  
(3) 0,1/2,1/2,1/2

(4) 4' (0,0,1/2) 1/2,0,z  
(4) 1/2,1/2,1/2

(5) 2' (0,1/2,0) 1/4,y,1/4  
(5) 1/2,1/2,1/2

(6) 2' (1/2,0,0) x,1/4,1/4  
(6) x,x,0

(7) 2' x,x,0  
(7) 0,0,0

(8) 2' x,x,0  
(8) 2,0,0

(9) T' 0,0,0  
(9) 1/2,1/2,1/2

(10) m' x,y,0  
(10) m,0,0

(11) 4' m' 1/2,0,z; 1/2,0,1/4  
(11) 1/2,1/2,1/2

(12) 4' m' 0,1/2,z; 0,1/2,1/4  
(12) 1/2,1/2,1/2

(13) n (1/2,0,1/2) x,1/4,z  
(13) m,0,0

(14) n (0,1/2,1/2) 1/4,y,z  
(14) 0,0,0

(15) m x,x,z  
(15) 0,0,0

(16) m x,x,z  
(16) 0,0,0
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) y + 1/2, x + 1/2, z + 1/2 [v,u,w]</td>
<td>(4) y + 1/2, x + 1/2, z + 1/2 [v,u,w]</td>
<td></td>
</tr>
<tr>
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<td>(5) x, y + 1/2, z + 1/2 [u,v,w]</td>
<td>(6) x, y + 1/2, z + 1/2 [u,v,w]</td>
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<tr>
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<td>(7) y, x, z [v,u,w]</td>
<td>(8) y, x, z [v,u,w]</td>
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<td>(9) x, y, z [u,v,w]</td>
<td>(10) x, y, z [u,v,w]</td>
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<td>(11) y + 1/2, x + 1/2, z + 1/2 [v,u,w]</td>
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<td>(13) x + 1/2, y + 1/2, z + 1/2 [u,v,w]</td>
<td>(14) x + 1/2, y + 1/2, z + 1/2 [u,v,w]</td>
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</tr>
<tr>
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<td>(15) y, x, z [v,u,w]</td>
<td>(16) y, x, z [v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

8 j ..m x,x,z [u,u,0]          x,x,z [u,u,0] |
|              | x + 1/2, x + 1/2, z + 1/2 [u,u,0] | x + 1/2, x + 1/2, z + 1/2 [u,u,0] |
|              | x + 1/2, x + 1/2, z + 1/2 [u,u,0] | x + 1/2, x + 1/2, z + 1/2 [u,u,0] |
|              | x,x,z [u,u,0] | x,x,z [u,u,0] |

8 i m'.. x,y,0 [u,v,0]          x,y,0 [u,v,0] |
|              | y + 1/2, x + 1/2, 1/2 [v,u,0] | y + 1/2, x + 1/2, 1/2 [v,u,0] |
|              | x + 1/2, y + 1/2, 1/2 [u,v,0] | x + 1/2, y + 1/2, 1/2 [u,v,0] |
|              | y,x,0 [v,u,0] | y,x,0 [v,u,0] |

8 h 2.. 0,1/2,z [0,0,w] 0,1/2,z + 1/2 [0,0,w] 1/2,0,z + 1/2 [0,0,w] 1/2,0,z [0,0,w] |
|              | 0,1/2,z [0,0,w] | 0,1/2,z [0,0,w] |
|              | 0,1/2,z [0,0,w] | 0,1/2,z [0,0,w] |

4 g m'.2m x, x,0 [u,u,0] x, x,0 [u,u,0] |
|              | x + 1/2, x + 1/2, 1/2 [u,u,0] | x + 1/2, x + 1/2, 1/2 [u,u,0] |

4 f m'.2m x,x,0 [u,u,0] x,x,0 [u,u,0] |
|              | x + 1/2, x + 1/2, 1/2 [u,u,0] | x + 1/2, x + 1/2, 1/2 [u,u,0] |

4 e 2.mm 0,0,z [0,0,0] 1/2,1/2, z + 1/2 [0,0,0] 1/2,1/2, z + 1/2 [0,0,0] 0,0,z [0,0,0] |

4 d 4'.. 0,1/2,1/4 [0,0,0] 0,1/2,3/4 [0,0,0] 1/2,0,1/4 [0,0,0] 1/2,0,3/4 [0,0,0] |

4 c 2/m'.. 0,1/2,0 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,0 [0,0,0] |

2 b m.mm 0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]
Symmetry of Special Projections

Along [0,0,1] p4gm  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,1/2,z

Along [1,0,0] \quad c_p \quad 2m'm'  
\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,0,0

Along [1,1,0] \quad p2mm1'  
\[ \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,0
**Origin** at center (mmm) at 2/m12/m

**Asymmetric unit**

\[0 \leq x \leq 1/2;\quad 0 \leq y \leq 1/2;\quad 0 \leq z \leq 1/2;\quad x \leq y\]

**Symmetry Operations**

1. \((1) \ 1\)
   
   \((1|0,0,0)\)

2. \((2) \ 2 \quad 0,0,z\)
   
   \((2z|0,0,0)\)

3. \((3) \ 4^{-} \ (0,0,1/2)\quad 0,1/2,z\)
   
   \((4z|1/2,1/2,1/2)\)

4. \((4) \ 4^{-} \ (0,0,1/2)\quad 1/2,0,z\)
   
   \((4z^{-1}|1/2,1/2,1/2)\)

5. \((5) \ 2' \ (0,1/2,0)\quad 1/4,y,1/4\)
   
   \((2y_1|1/2,1/2,1/2)\)

6. \((6) \ 2' \ (1/2,0,0)\quad x,1/4,1/4\)
   
   \((2xy_0|0,0,0)\)

7. \((7) \ 2 \quad x,x,0\)
   
   \((2xy|0,0,0)\)

8. \((8) \ 2 \quad x,x,0\)
   
   \((2xy_0|0,0,0)\)

9. \((9) \ 1 \quad 0,0,0\)
   
   \((1|0,0,0)\)

10. \((10) \ m \quad x,y,0\)
    
    \((mz_0|0,0,0)\)

11. \((11) \ 4^{-} \quad 1/2,0,z;\quad 1/2,0,1/4\)
    
    \((4z|1/2,1/2,1/2)\)

12. \((12) \ 4^{-} \quad 0,1/2,z;\quad 0,1/2,1/4\)
    
    \((4z^{-1}|1/2,1/2,1/2)\)

13. \((13) \ n' \ (1/2,0,1/2)\quad x,1/4,z\)
    
    \((mz_1|1/2,1/2,1/2)\)

14. \((14) \ n' \ (0,1/2,1/2)\quad 1/4,y,z\)
    
    \((mxy_0|0,0,0)\)

15. \((15) \ m \quad x,x,z\)
    
    \((mxy|0,0,0)\)

16. \((16) \ m \quad x,x,z\)
    
    \((mxy_0|0,0,0)\)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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2  a  m.mm  0,0,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4gm1’

\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]

Origin at 0,1/2,z

Along [1,0,0] c2’mm’

\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \]

Origin at x,0,0

Along [1,1,0] p2mm1’

\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]

Origin at x,x,0
Origin at center (m'm'm) at 2/m12'/m'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2z | 0,0,0)

(3) 4 ' (0,0,1/2) 0,1/2,z
(4z | 1/2,1/2,1/2)'

(4) 4 ' (0,0,1/2) 1/2,0,z
(4z | 1/2,1/2,1/2)'

(5) 2 (0,1/2,0) 1/4,y,1/4
(2z | 1/2,1/2,1/2)

(6) 2 (1/2,0,0) x,1/4,1/4
(2z | 1/2,1/2,1/2)

(7) 2' x,x,0
(2xy | 0,0,0)'

(8) 2' x,x,0
(2xy | 0,0,0)'

(9) $\bar{1}$ 0,0,0
(1 | 0,0,0)

(10) m x,y,0
(mz | 0,0,0)

(11) $\bar{4}$ ' (1/2,0,z) 1/2,0,1/4
(4z | 1/2,1/2,1/2)'

(12) $\bar{4}$ ' (1/2,0,z) 0,1/2,1/4
(4z | 1/2,1/2,1/2)'

(13) n (1/2,0,1/2) x,1/4,z
(mz | 1/2,1/2,1/2)

(14) n (0,1/2,1/2) 1/4,y,z
(mz | 1/2,1/2,1/2)

(15) m' x,x,z
(mxy | 0,0,0)'

(16) m' x,x,z
(mxy | 0,0,0)'

P4_1/mnm' 4'/mmm'

Tetragonal

136.5.1156 P4_1/m2_/n2'/m'
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
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<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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</table>
Symmetry of Special Projections

Along \([0,0,1]\) p4gm1'

\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at \(0,1/2,z\)

Along \([1,0,0]\) \(c'2mm'\)

\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at \(x,0,0\)

Along \([1,1,0]\) p2'\(\bar{m}\)m'

\[ \mathbf{a}^* = -\mathbf{c} \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]
Origin at \(x,x,0\)
P4₁/m'2/m'2/m

Tetragonal

136.6.1157

4'/m'm'm

Origin at center (mmm') at 2/m'12'/m

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ y

Symmetry Operations

(1) 1
(1 | 0,0,0)

(5) 2 (0,1/2,0) 1/4,y,1/4
(2z | 1/2,1/2,1/2)

(9) T' 0,0,0
(1 | 0,0,0)'

(13) n' (1/2,0,1/2) x,1/4,z
(my | 1/2,1/2,1/2)'

(2) 2' 0,0,z
(2'z | 0,0,0)

(6) 2 (1/2,0,0) x,1/4,1/4
(2'z | 1/2,1/2,1/2)

(10) m' x,y,0
(m | 0,0,0)'

(11) 4' 1/2,0,z; 1/2,0,1/4
(4z | 1/2,1/2,1/2)

(14) n' (0,1/2,1/2) 1/4,y,z
(m'y | 1/2,1/2,1/2)'

(3) 4' (0,0,1/2) 0,1/2,z
(4z | 1/2,1/2,1/2)'

(4) 4' (0,0,1/2) 1/2,0,z
(4z | 1/2,1/2,1/2)'

(7) 2' x,x,0
(2'y | 0,0,0)'

(12) 4' - 0,1/2,z; 0,1/2,1/4
(4z | -1/2,1/2,1/2)

(8) 2' x,x,0
(2'y | 0,0,0)'

(15) m x,x,z
(m | 0,0,0)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<td>2</td>
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Continued

Symmetry of Special Projections

Along [0,0,1] p4'g'm
\[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,1/2,z

Along [1,0,0] c 2m'm'
\[ \mathbf{a}^* = \mathbf{b}, \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,0,0

Along [1,1,0] p2mm1'
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2, \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,0

2 a m'.mm 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]
**Origin** at center (m'm'm') at 2/m12'/m'

**Asymmetric unit**

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y
\]

**Symmetry Operations**

1. 1
   - (1) 1
     - (1|0,0,0)

2. 2
   - (2) 2 0,0,z
     - (2\text{_z}|0,0,0)

3. 4\text{~}
   - (3) 4\text{~} (0,0,1/2) 0,1/2,z
     - (4\text{~}_z|1/2,1/2,1/2)

4. 4
   - (4) 4 (0,0,1/2) 1/2,0,z
     - (4\text{~}_z|1/2,1/2,1/2)

5. 2' (0,1/2,0) 1/4,y,1/4
   - (5) 2' (0,1/2,0) 1/4,y,1/4
     - (2\text{z}_y|0,0,0)

6. 2' (1/2,0,0) x,1/4,1/4
   - (6) 2' (1/2,0,0) x,1/4,1/4
     - (2\text{z}_y|0,0,0)

7. 2' x,x,0
   - (7) 2' x,x,0
     - (2\text{z}_y|0,0,0)

8. 2' x,x,0
   - (8) 2' x,x,0
     - (2\text{z}_y|0,0,0)

9. 1/2,0,0
   - (9) 1/2,0,0
     - (1|0,0,0)

10. m x,y,0
    - (10) m x,y,0
      - (m_z|0,0,0)

11. 4\text{~}
    - (11) 4\text{~} (1/2,0,1/2) z,1/2,0,1/4
      - (4\text{~}_z|1/2,1/2,1/2)

12. 4\text{~}
    - (12) 4\text{~} (1/2,0,1/2) z,1/2,0,1/4
      - (4\text{~}_z|1/2,1/2,1/2)

13. n' (1/2,0,1/2) x,1/4,z
    - (13) n' (1/2,0,1/2) x,1/4,z
      - (m_y|1/2,1/2,1/2)

14. n' (0,1/2,1/2) 1/4,y,z
    - (14) n' (0,1/2,1/2) 1/4,y,z
      - (m_y|0,0,0)

15. m' x,x,z
    - (15) m' x,x,z
      - (m_y|0,0,0)

16. m' x,x,z
    - (16) m' x,x,z
      - (m_y|0,0,0)
### Generators selected

(1); \( t(1,0,0) \); \( t(0,1,0) \); \( t(0,0,1) \); (2); (3); (5); (9).

### Positions

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<tr>
<td>16 k 1</td>
<td>(1) ( x,y,z, [u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(3) ( \bar{y} + 1/2, x + 1/2, z + 1/2, [\bar{v}, u, w] )</td>
</tr>
<tr>
<td></td>
<td>(5) ( \bar{x} + 1/2, y + 1/2, z + 1/2, [u, \bar{v}, w] )</td>
</tr>
<tr>
<td></td>
<td>(7) ( y, x, \bar{z}, [v, \bar{u}, w] )</td>
</tr>
<tr>
<td></td>
<td>(9) ( x, y, \bar{z}, [u, v, w] )</td>
</tr>
<tr>
<td></td>
<td>(11) ( y + 1/2, x + 1/2, z + 1/2, [v, u, w] )</td>
</tr>
<tr>
<td></td>
<td>(13) ( x + 1/2, y + 1/2, z + 1/2, [u, \bar{v}, w] )</td>
</tr>
<tr>
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<td>(15) ( y, x, z, [v, u, w] )</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>8 j ..m'</th>
<th>x, x, z [u, u, w]</th>
<th>( x, \bar{x}, z [u, \bar{u}, w] )</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>( \bar{x} + 1/2, x + 1/2, z + 1/2, [u, u, w] )</td>
<td>( x + 1/2, \bar{x} + 1/2, z + 1/2, [\bar{u}, u, w] )</td>
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<td>( \bar{x} + 1/2, x + 1/2, \bar{z} + 1/2, [u, u, w] )</td>
<td>( x + 1/2, \bar{x} + 1/2, \bar{z} + 1/2, [\bar{u}, u, w] )</td>
</tr>
<tr>
<td></td>
<td>( x, x, z, [u, u, w] )</td>
<td>( \bar{x}, \bar{x}, z [u, \bar{u}, w] )</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>8 i m..</th>
<th>x, y, 0 [0, 0, w]</th>
<th>( \bar{x}, \bar{y}, 0 [0, 0, w] )</th>
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<tbody>
<tr>
<td></td>
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<td>( y + 1/2, \bar{x} + 1/2, 1/2, [0, 0, w] )</td>
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<tr>
<td></td>
<td>( \bar{x} + 1/2, y + 1/2, 1/2, [0, 0, w] )</td>
<td>( x + 1/2, \bar{y} + 1/2, 1/2, [0, 0, w] )</td>
</tr>
<tr>
<td></td>
<td>( y, x, 0 [0, 0, w] )</td>
<td>( \bar{y}, x, 0 [0, 0, w] )</td>
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<table>
<thead>
<tr>
<th>8 h 2..</th>
<th>0, 1/2, z [0, 0, w]</th>
<th>( 0, 1/2, z + 1/2, [0, 0, w] )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0, 1/2, ( \bar{z} ) [0, 0, w]</td>
<td>( 1/2, 0, \bar{z} + 1/2, [0, 0, w] )</td>
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<tr>
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<td>0, 1/2, ( \bar{z} + 1/2 ) [0, 0, w]</td>
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<tr>
<td></td>
<td>0, 1/2, ( \bar{z} + 1/2 ) [0, 0, w]</td>
<td>( 0, 1/2, z + 1/2, [0, 0, w] )</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>4 g m.2' ( \text{m}' )</th>
<th>x, ( \bar{x}, \bar{x} ) [0, 0, w]</th>
<th>( x, x, 0 [0, 0, w] )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \bar{x} + 1/2, x + 1/2, 1/2, [0, 0, w] )</td>
<td>( x + 1/2, \bar{x} + 1/2, 1/2, [0, 0, w] )</td>
</tr>
<tr>
<td></td>
<td>( \bar{x} + 1/2, x + 1/2, 1/2, [0, 0, w] )</td>
<td>( x + 1/2, \bar{x} + 1/2, 1/2, [0, 0, w] )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4 f m.2' ( \text{m}' )</th>
<th>x, x, 0 [0, 0, w]</th>
<th>( \bar{x}, \bar{x}, 0 [0, 0, w] )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \bar{x} + 1/2, x + 1/2, 1/2, [0, 0, w] )</td>
<td>( x + 1/2, \bar{x} + 1/2, 1/2, [0, 0, w] )</td>
</tr>
<tr>
<td></td>
<td>( \bar{x} + 1/2, x + 1/2, 1/2, [0, 0, w] )</td>
<td>( x + 1/2, \bar{x} + 1/2, 1/2, [0, 0, w] )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4 e 2.m ( \text{m}' )</th>
<th>0, 0, z [0, 0, w]</th>
<th>( 1/2, 1/2, z + 1/2, [0, 0, w] )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( 1/2, 1/2, z + 1/2, [0, 0, w] )</td>
<td>( 1/2, 1/2, \bar{z} + 1/2, [0, 0, w] )</td>
</tr>
<tr>
<td></td>
<td>( 0, 0, \bar{z} [0, 0, w] )</td>
<td>( 0, 0, \bar{z} [0, 0, w] )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4 d 4..</th>
<th>0, 1/2, 1/4 [0, 0, w]</th>
<th>( 0, 1/2, 3/4, [0, 0, w] )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( 1/2, 0, 1/4 [0, 0, w] )</td>
<td>( 1/2, 0, 3/4 [0, 0, w] )</td>
</tr>
<tr>
<td></td>
<td>( 1/2, 0, 1/2 [0, 0, w] )</td>
<td>( 1/2, 0, 0 [0, 0, w] )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4 c 2/m..</th>
<th>0, 1/2, 0 [0, 0, w]</th>
<th>( 1/2, 1/2, 0 [0, 0, w] )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( 1/2, 0, 0 [0, 0, w] )</td>
<td>( 1/2, 0, 0 [0, 0, w] )</td>
</tr>
</tbody>
</table>

| 2 b m.m \( \text{m}' \) | 0, 0, 1/2 [0, 0, w] | \( 1/2, 1/2, 0 [0, 0, w] \) |
2  a  m.m'm'  0,0,0 [0,0,w]  1/2,1/2,1/2 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p4gm1'  
\[a^* = a, \quad b^* = b\]
Origin at 0,1/2,z

Along [1,0,0] c2mm  
\[a^* = b, \quad b^* = c\]
Origin at x,0,0

Along [1,1,0] p2'mm'  
\[a^* = -c, \quad b^* = (-a + b)/2\]
Origin at x,x,0
Origin at center (m'm'm') at 2/m'12/m'

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x < y

Symmetry Operations

(1) 1 (1 | 0,0,0)
(2) 2 0,0,z (2z | 0,0,0)
(3) 4' + (0,0,1/2) 0,1/2,z (4z | 1/2,1/2,1/2')
(4) 4' - (0,0,1/2) 1/2,0,z (4z^-1 | 1/2,1/2,1/2')
(5) 2' (0,1/2,0) 1/4,y,1/4 (2y | 1/2,1/2,1/2')
(6) 2' (1/2,0,0) x,1/4,1/4 (2x | 1/2,1/2,1/2')
(7) 2 x,x,0 (2y | 0,0,0)
(8) 2 x,x,0 (2y | 0,0,0)
(9) T | 0,0,0'
(10) m' x,y,0 (mz | 0,0,0')
(11) 4' + 1/2,0,z; 1/2,0,1/4 (4z^-1 | 1/2,1/2,1/2)
(12) 4' - 0,1/2,z; 0,1/2,1/4 (4z^-1 | 1/2,1/2,1/2)
(13) n (1/2,0,1/2) x,1/4,z (mz | 1/2,1/2,1/2)
(14) n (0,1/2,1/2) 1/4,y,z (mz | 1/2,1/2,1/2)
(15) m' x,x,z (mz | 0,0,0')
(16) m' x,x,z (mz | 0,0,0')
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 16  k 1                                    | (1) x,y,z [u,v,w]  
(2) x',y',z [u',v',w]  
(3) y+1/2,x+1/2,z+1/2 [v,u,w]  
(4) y+1/2,x+1/2,z+1/2 [v,u,w]  
(5) x+1/2,y+1/2,z+1/2 [u,v,w]  
(6) x+1/2,y+1/2,z+1/2 [u,v,w]  
(7) y,x,z [v,u,w]  
(8) y,x,z [v,u,w]  
(9) x,y,z [u,v,w]  
(10) x,y,z [u,v,w]  
(11) y+1/2,x+1/2,z+1/2 [v,u,w]  
(12) y+1/2,x+1/2,z+1/2 [v,u,w]  
(13) x+1/2,y+1/2,z+1/2 [u,v,w]  
(14) x+1/2,y+1/2,z+1/2 [u,v,w]  
(15) y,x,z [v,u,w]  
(16) y,x,z [v,u,w] |
| 8  j  ..m'                                 | x,x,z [u,u,w]  
x+1/2,x+1/2,z+1/2 [u,u,w]  
x+1/2,x+1/2,z+1/2 [u,u,w]  
x+1/2,x+1/2,z+1/2 [u,u,w]  
x+1/2,x+1/2,z+1/2 [u,u,w]  
x,x,z [u,u,w]  
x,x,z [u,u,w] |
| 8  i  m'..                                 | x,y,0 [u,v,0]  
 y+1/2,x+1/2,1/2 [v,u,0]  
x+1/2,y+1/2,1/2 [u,v,0]  
y,x,0 [u,v,0]  
y,x,0 [u,v,0]  
y,x,0 [u,v,0] |
| 8  h  2..                                  | 0,1/2,z [0,0,w]  
0,1/2,z [0,0,w]  
0,1/2,z [0,0,w]  
0,1/2,z [0,0,w]  
0,1/2,z [0,0,w]  
1/2,0,z+1/2 [0,0,w]  
1/2,0,z+1/2 [0,0,w]  
1/2,0,z+1/2 [0,0,w]  
1/2,0,z+1/2 [0,0,w]  
1/2,0,z+1/2 [0,0,w]  
1/2,0,z+1/2 [0,0,w] |
| 4  g  m'.2m'                               | x,x,0 [u,u,0]  
x,x,0 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0] |
| 4  f  m'.2m'                               | x,x,0 [u,u,0]  
x,x,0 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0]  
x+1/2,x+1/2,1/2 [u,u,0] |
| 4  e  2.m'm'                                | 0,0,z [0,0,w]  
1/2,1/2,z+1/2 [0,0,w]  
1/2,1/2,z+1/2 [0,0,w]  
1/2,1/2,z+1/2 [0,0,w]  
1/2,1/2,z+1/2 [0,0,w]  
0,0,z [0,0,w]  
0,0,z [0,0,w] |
| 4  d  4..                                  | 0,1/2,1/4 [0,0,w]  
0,1/2,1/4 [0,0,w]  
0,1/2,1/4 [0,0,w]  
0,1/2,1/4 [0,0,w]  
1/2,0,1/4 [0,0,w]  
1/2,0,1/4 [0,0,w]  
1/2,0,1/4 [0,0,w] |
| 4  c  2/m'..                                | 0,1/2,0 [0,0,0]  
0,1/2,1/2 [0,0,0]  
0,1/2,1/2 [0,0,0]  
0,1/2,1/2 [0,0,0]  
1/2,0,1/2 [0,0,0]  
1/2,0,1/2 [0,0,0]  
1/2,0,1/2 [0,0,0] |
| 2  b  m'.m'm'                               | 0,0,1/2 [0,0,0]  
1/2,1/2,0 [0,0,0]  
1/2,1/2,0 [0,0,0]  
1/2,1/2,0 [0,0,0]  
1/2,1/2,0 [0,0,0]  
1/2,1/2,0 [0,0,0]  
1/2,1/2,0 [0,0,0] |
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry Group</th>
<th>Relations</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4'gm'</td>
<td>$a^* = a$</td>
<td>0,1/2,z</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b$</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>c$_p$: 2m'm'</td>
<td>$a^* = b$</td>
<td>x,0,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = c$</td>
<td></td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p2m'm'</td>
<td>$a^* = (-a + b)/2$</td>
<td>x,x,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = c$</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at center (m'm'm') at 2/m'12/m'

**Asymmetric unit**
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x < y \]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(1 | 0,0,0) & \\
(5) & \quad 2 \ (0,1/2,0) \quad 1/4,y,1/4 \\
& \quad (2_z | 1/2,1/2,1/2) \\
(9) & \quad \bar{1} \quad 0,0,0 \\
& \quad (\bar{1} | 0,0,0)' \\
(13) & \quad n' \ (1/2,0,1/2) \quad x,1/4,z \\
& \quad (m_y | 1/2,1/2,1/2)' \\
(14) & \quad n' \ (0,1/2,1/2) \quad 1/4,y,z \\
& \quad (m_z | 1/2,1/2,1/2)' \\
(15) & \quad m' \quad x,1/4,z \\
& \quad (m_x | 0,0,0)' \\
(16) & \quad m' \quad x,y,z \\
& \quad (m_y | 0,0,0)' \\
\end{align*}
\]
### Generators selected

\[ (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9). \]

### Positions

**Multiplicities, Wyckoff letters, Site Symmetries.**

<table>
<thead>
<tr>
<th>Number</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>1</td>
<td>k</td>
<td>1</td>
</tr>
<tr>
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<td>1</td>
<td>j</td>
<td>0.5</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>i</td>
<td>0.5</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>h</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>g</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>f</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>e</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>d</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>c</td>
<td>0.5</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>b</td>
<td>0.5</td>
</tr>
</tbody>
</table>

**Coordinates**

1. \((1) x, y, z \) \([u, v, w]\)
2. \((2) x, y, z \) \([u, v, w]\)
3. \((3) y + 1/2, x + 1/2, z + 1/2 \) \([v, u, w]\)
4. \((4) x + 1/2, y + 1/2, z + 1/2 \) \([u, v, w]\)
5. \((5) y, x, z \) \([v, u, w]\)
6. \((6) x, y, z \) \([u, v, w]\)
7. \((7) y + 1/2, x, z + 1/2 \) \([v, u, w]\)
8. \((8) y, x, z \) \([v, u, w]\)
9. \((9) x, y, z \) \([u, v, w]\)
10. \((10) y, x + 1/2, z + 1/2 \) \([u, v, w]\)
11. \((11) y + 1/2, x + 1/2, z + 1/2 \) \([v, u, w]\)
12. \((12) y, x + 1/2, z + 1/2 \) \([v, u, w]\)
13. \((13) x + 1/2, y + 1/2, z + 1/2 \) \([u, v, w]\)
14. \((14) x, y + 1/2, z + 1/2 \) \([u, v, w]\)
15. \((15) y, x + 1/2, z + 1/2 \) \([u, v, w]\)
16. \((16) y, x, z \) \([v, u, w]\)
Symmetry of Special Projections

Along [0,0,1] p4g'm'  
\(a^* = a\)  \(b^* = b\)  
Origin at 0,1/2,z

Along [1,0,0] c2m'm'  
\(a^* = b\)  \(b^* = c\)  
Origin at x,0,0

Along [1,1,0] p2m'm'  
\(a^* = (-a + b)/2\)  \(b^* = c\)  
Origin at x,x,0
Origin at $\bar{4}$m2/n, at -1/4,1/4,-1/4 from 1

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1

(1) 0,0,0

(2) 2 0,0,z

(2) $z|0,0,0$

(3) 4+ (0,0,1/2) 0,1/2,z

(3) $4|z_1/2,1/2,1/2$

(4) 4+ (0,0,1/2) 1/2,0,z

(4) $4|z_1/2,1/2,1/2$

(5) 2 (0,1/2,0) 1/4,y,1/4

(5) $2|1/2,1/2,1/2$

(6) 2 (1/2,0,0) x,1/4,1/4

(6) $2_{xy}|0,0,0$

(7) 2 x,x,0

(7) $2_{xy}|0,0,0$

(8) 2 x,x,0

(8) $2_{xy}|0,0,0$

(9) $\bar{4}$ 1/4,1/4,1/4

(9) $1/2,1/2,1/2$

(10) n (1/2,1/2,0) x,y,1/4

(10) $m_{xy}|1/2,1/2,1/2$

(11) $\bar{4}|z_1/2,0,0$

(11) $\bar{4}|z_0,0,0$

(12) $\bar{4}$ 0,0,z; 0,0,0

(12) $\bar{4}|z_0,0,0$

(13) m x,z

(13) $m_{xy}|0,0,0$

(14) m 0,y,z

(14) $m_{xy}|0,0,0$

(15) c (0,0,1/2) x+1/2,x,z

(15) $m_{xy}|1/2,1/2,1/2$

(16) n (1/2,1/2,1/2) x,x,z

(16) $m_{xy}|1/2,1/2,1/2$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

## Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>16</td>
<td>h</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(7) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(8) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(9) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(10) y,x,z [v,u,w]</td>
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<td>(11) y,x,z [v,u,w]</td>
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<td>(12) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(13) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
</tr>
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<td>(14) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
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<td></td>
<td>(15) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>.m.</td>
<td>0,y,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>y+1/2,1/2,z+1/2 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,y+1/2,z+1/2 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,y+1/2,z+1/2 [0,u,0]</td>
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<tr>
<td>8</td>
<td>f</td>
<td>x,x,0 [u,u,0]</td>
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<td>.2</td>
<td>x,x,0 [u,u,0]</td>
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<td>x+1/2,x+1/2,z+1/2 [u,u,0]</td>
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<td>x+1/2,x+1/2,z+1/2 [u,u,0]</td>
</tr>
<tr>
<td>8</td>
<td>e</td>
<td>1/4,1/4,1/4 [u,v,w]</td>
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<tr>
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<td>1</td>
<td>3/4,3/4,1/4 [u,v,w]</td>
</tr>
<tr>
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<td></td>
<td>1/4,3/4,3/4 [v,u,w]</td>
</tr>
<tr>
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<td>3/4,1/4,3/4 [v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>2mm</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,0,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>2mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>4m2</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>4m2</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>4m'</td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p2mg1'</td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>p2a</td>
</tr>
<tr>
<td>[0,0,1]</td>
<td>p2a</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
Origin at x,1/4,1/4
Origin at x,x,0
Origin at \( \overline{4} m2/n1' \), at \(-1/4,1/4,-1/4\) from \( \overline{1} 1' \)

Asymmetric unit \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4 \)

Symmetry Operations

For \( 1 + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(1 | 0,0,0) \\
(5) & \quad 2 \quad (0,1/2,0) \\
(2y | 1/2,1/2,1/2) \\
(9) & \quad \overline{1} \quad 1/4,1/4,1/4 \\
(1/2,1/2,1/2) \\
(13) & \quad m \quad x,0,z \\
(m | 0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2z | 0,0,0) \\
(6) & \quad 2 \quad (1/2,0,0) \\
(2x | 1/2,1/2,1/2) \\
(10) & \quad n \quad (1/2,1/2,0) \\
(x,y,1/4) \\
(3) & \quad 4^+ \quad (0,0,1/2) \\
(4_x | 1/2,1/2,1/2) \\
(4) & \quad 4^- \quad (0,0,1/2) \\
(4_z \overline{1} | 1/2,1/2,1/2) \\
(7) & \quad 2 \quad x,x,0 \\
(2_{xy} | 0,0,0) \\
(8) & \quad 2 \quad x,x,0 \\
(2_{xy} | 0,0,0) \\
(11) & \quad 4^+ \quad 0,0,z; \quad 0,0,0 \\
(4_z | 0,0,0) \\
(12) & \quad 4^- \quad 0,0,z; \quad 0,0,0 \\
(4_z \overline{1} | 0,0,0) \\
(14) & \quad m \quad 0,y,z \\
(m_y | 0,0,0) \\
(15) & \quad c \quad (0,0,1/2) \\
(x+1/2,\overline{x},z) \\
(3) & \quad 4^+ \quad (0,0,1/2) \\
(4_x | 1/2,1/2,1/2) \\
(16) & \quad n \quad (1/2,1/2,1/2) \\
(x,x,z) \\
(2_{xy} | 0,0,0)
\end{align*}
\]
Continued

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Coordinates</td>
</tr>
<tr>
<td></td>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
</tr>
</tbody>
</table>

**For 1' + set**

1. \( t'(1,0,0); t(0,1,0); t(0,0,1); \)
2. \( 1'(2); (3); (5); (9); \)

### Generators selected

- (1); \( t(1,0,0); t(0,1,0); t(0,0,1) \)
- (2); (3); (5); (9); 1'.

### Positions

#### Coordinates

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 h 11'</td>
</tr>
<tr>
<td>(1) ( x,y,z [0,0,0] )</td>
</tr>
<tr>
<td>(2) ( x,y,z [0,0,0] )</td>
</tr>
<tr>
<td>(3) ( \bar{y}+1/2,x+1/2,z+1/2 [0,0,0] )</td>
</tr>
<tr>
<td>(4) ( y+1/2,x+1/2,z+1/2 [0,0,0] )</td>
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<td>(12) ( y,x,z [0,0,0] )</td>
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<tr>
<td>(14) ( x,y,z [0,0,0] )</td>
</tr>
<tr>
<td>(15) ( y+1/2,x+1/2,z+1/2 [0,0,0] )</td>
</tr>
<tr>
<td>(16) ( y+1/2,x+1/2,z+1/2 [0,0,0] )</td>
</tr>
</tbody>
</table>

| 8 g .m.1' |
| 0,y,z [0,0,0] |
| 0,y,z [0,0,0] |
| \( \bar{y}+1/2,1/2,z+1/2 [0,0,0] \) |
| \( y+1/2,1/2,z+1/2 [0,0,0] \) |
| 1/2,y+1/2,z+1/2 [0,0,0] |
| 1/2,y+1/2,z+1/2 [0,0,0] |
| \( y,0,z [0,0,0] \) |
| \( y,0,z [0,0,0] \) |
| \( \bar{y},0,z [0,0,0] \) |
| \( \bar{y},0,z [0,0,0] \) |

| 8 f .21' |
| x,x,0 [0,0,0] |
| x,x,0 [0,0,0] |
| \( \bar{x}+1/2,x+1/2,1/2 [0,0,0] \) |
| \( x+1/2,\bar{x}+1/2,1/2 [0,0,0] \) |
| \( x+1/2,\bar{x}+1/2,1/2 [0,0,0] \) |
| \( x+1/2,\bar{x}+1/2,1/2 [0,0,0] \) |
| \( x,0 [0,0,0] \) |
| \( x,0 [0,0,0] \) |

| 8 e 11' |
| 1/4,1/4,1/4 [0,0,0] |
| 3/4,3/4,3/4 [0,0,0] |
| 1/4,3/4,3/4 [0,0,0] |
| 3/4,1/4,3/4 [0,0,0] |
| 1/4,3/4,3/4 [0,0,0] |
| 3/4,1/4,3/4 [0,0,0] |

| 4 d 2mm.1' |
| 0,1/2,z [0,0,0] |
| 0,1/2,z+1/2 [0,0,0] |
| 1/2,0,z+1/2 [0,0,0] |
| 1/2,0,z+1/2 [0,0,0] |

| 4 c 2mm.1' |
| 0,0,z [0,0,0] |
| 1/2,1/2,z+1/2 [0,0,0] |
| 1/2,1/2,z+1/2 [0,0,0] |
| 0,0,z [0,0,0] |

| 2 b 4m21' |
| 0,0,1/2 [0,0,0] |
| 1/2,1/2,0 [0,0,0] |
| 137.2.1162 - 2 - 2444 |
Continued

Symmetry of Special Projections

Along [0,0,1] p4mm1'
\[ a^* = \frac{a - b}{2}, \ b^* = \frac{a + b}{2} \]
Origin at 0,0,z

Along [1,0,0] p2mg1'
\[ a^* = b, \ b^* = c \]
Origin at x,1/4,1/4

Along [1,1,0] p2mm1'
\[ a^* = \frac{-a + b}{2}, \ b^* = \frac{c}{2} \]
Origin at x,x,0

2 a 4m21' 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]
Origin at $\overline{4}m2'/n$, at -1/4,1/4,-1/4 from 1'.

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

1. $1$
   - $(1|0,0,0)$

2. $2' \ 0,0,z$
   - $(2_x|0,0,0)$

3. $4' (0,0,1/2) \ 0,1/2,z$
   - $(4_z|1/2,1/2,1/2)$

4. $4' (0,0,1/2) \ 1/2,0,z$
   - $(4_z^{-1}|1/2,1/2,1/2)$

5. $2' (0,1/2,0) \ 1/4,y,1/4$
   - $(2_z|1/2,1/2,1/2)'$

6. $2' (1/2,0,0) \ x,1/4,1/4$
   - $(2_y|0,0,0)'$

7. $2' \ x,x,0$
   - $(2_{xy}|0,0,0)'$

8. $2' \ x,x,0$
   - $(2_{xy}|0,0,0)'$

9. $\overline{1} \ 1/4,1/4,1/4$
   - $(\overline{1}|1/2,1/2,1/2)'$

10. $n' (1/2,1/2,0) \ x,y,1/4$
    - $(m_z|1/2,1/2,1/2)'$

11. $\overline{4} \ 0,0,z; \ 0,0,0$
    - $(\overline{4}_z|0,0,0)'$

12. $\overline{4} \ 0,0,z; \ 0,0,0$
    - $(\overline{4}_z^{-1}|0,0,0)'$

13. $m \ x,0,z$
    - $(m_{xy}|0,0,0)$

14. $m \ 0,y,z$
    - $(m_{xy}|0,0,0)$

15. $c (0,0,1/2) \ x+1/2,x,z$
    - $(m_{xy}|1/2,1/2,1/2)$

16. $n (1/2,1/2,1/2) \ x,x,z$
    - $(m_{xy}|1/2,1/2,1/2)$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
<td>.m.</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>..2'</td>
</tr>
<tr>
<td>8</td>
<td>e</td>
<td>1'</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>2mm.</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>2mm.</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4'm2'</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4'm2'</td>
</tr>
</tbody>
</table>

**Coordinates**

<table>
<thead>
<tr>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) y+1/2,x+1/2,z+1/2 [u,v,w]</th>
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<th>(8) y,x,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,y,z [u,0,0]</td>
<td>1/2,y,z+1/2 [0,0,0]</td>
<td>1/2,y+1/2,z+1/2 [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
<td>0,y,z [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm</th>
<th>Along [1,0,0] p2mg1'</th>
<th>Along [1,1,0] p2a 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>a* = b</td>
<td>a* = -c/2</td>
</tr>
<tr>
<td>b* = (a + b)/2</td>
<td>b* = c</td>
<td>b* = (-a + b)/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,1/4,1/4

Origin at x,x,0
Origin at $\bar{4}m'n$, at $-1/4,1/4,-1/4$ from $\bar{1}$

Asymmetric unit $\quad 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
     (1 0 0, 0, 0)

(2) 2 0, 0, z
     (2z 0, 0, 0)

(3) $4^+ \cdot (0,0,1/2) \quad 0,1/2,z$
     ($4_z 1/2,1/2,1/2'$)

(4) $4^- \cdot (0,0,1/2) \quad 1/2,0,z$
     ($4_{z^-} 1/2,1/2,1/2'$)

(5) $2' \cdot (0,1/2,0) \quad 1/4, y, 1/4$
     ($2_y 1/2,1/2,1/2'$)

(6) $2' \cdot (1/2,0,0) \quad x, 1/4, 1/4$
     ($2_{xy} 0, 0, 0$)

(7) $2 \cdot x, x, 0$
     ($2_{xy} 0, 0, 0$)

(8) $2 \cdot x, x, 0$
     ($2_{xy} 0, 0, 0$)

(9) $\bar{1} \cdot 1/4,1/4,1/4$
     ($\bar{1} 1/2,1/2,1/2$)

(10) n (1/2,1/2,0) \quad x, y, 1/4
      (m_{xy} 1/2,1/2,1/2)

(11) $\overline{4}^+ \cdot 0,0,z; 0,0,0$
      ($\overline{4}_z 0,0,0$)

(12) $\overline{4}^- \cdot 0,0,z; 0,0,0$
      ($\overline{4}_{z^-} 0,0,0$)

(13) $m' \cdot x, 0, z$
     (m_{x} 0, 0, 0)

(14) $m' \cdot 0, y, z$
     (m_{y} 0, 0, 0)

(15) $c \cdot (0,0,1/2) \quad x+1/2, x, z$
     ($m_{xy} 1/2,1/2,1/2$)

(16) n (1/2,1/2,1/2) \quad x, x, z
     ($m_{xy} 1/2,1/2,1/2$)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 h 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [v,u,w] (3) y+1/2,x+1/2,z+1/2 [v,u,w] (4) y+1/2,x+1/2,z+1/2 [v,u,w] (5) x+1/2,y+1/2,z+1/2 [u,v,w] (6) x+1/2,y+1/2,z+1/2 [u,v,w] (7) y+1/2,x+1/2,z+1/2 [v,u,w] (8) y+1/2,x+1/2,z+1/2 [v,u,w] (9) y+1/2,x+1/2,z+1/2 [v,u,w] (10) y+1/2,x+1/2,z+1/2 [v,u,w] (11) y+1/2,x+1/2,z+1/2 [v,u,w] (12) y+1/2,x+1/2,z+1/2 [v,u,w] (13) y+1/2,x+1/2,z+1/2 [v,u,w] (14) y+1/2,x+1/2,z+1/2 [v,u,w] (15) y+1/2,x+1/2,z+1/2 [v,u,w] (16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_0, 4m'm'  
along [1,0,0] p_2'm'g  
along [1,1,0] p_2a, 2m'm'

a^* = (a - b)/2  
b^* = (a + b)/2
**Origin** at $\overline{4}m2'n'$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from $\overline{1}$

**Asymmetric unit**

$0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq \frac{1}{4}$

**Symmetry Operations**

1. $(1) \ 1$
   
2. $(2) \ 2 \ 0,0,z$
   
3. $(3) \ 4' \cdot (0,0,1/2) \ 0,1/2,z$
   
4. $(4) \ 4' \cdot (0,0,1/2) \ 1/2,0,z$
   
5. $(5) \ 2 \ (0,1/2,0) \ 0,0,0$

6. $(6) \ 2 \ (1/2,0,0) \ x,1/4,1/4$

7. $(7) \ 2' \ x,x,0$

8. $(8) \ 2' \ x,x,0$

9. $(9) \ \overline{1} \ 1/4,1/4,1/4$

10. $(10) \ n \ (1/2,1/2,0) \ x,y,1/4$

11. $(11) \ 4 \cdot \ 0,0,z; 0,0,0$

12. $(12) \ 4 \cdot \ 0,0,z; 0,0,0$

13. $(13) \ m \ x,0,z$

14. $(14) \ m \ 0,y,z$

15. $(15) \ c' \ (0,0,1/2) \ x+1/2,x,z$

16. $(16) \ n' \ (1/2,1/2,1/2) \ x,x,z$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>16 h 1</td>
<td>(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]</td>
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<td>4 d 2mm.</td>
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<td>1/2,0,z+1/2 [0,0,0] 1/2,0,z+1/2 [0,0,0]</td>
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<tr>
<td>4 c 2mm.</td>
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<tr>
<td>2 b 4'm2'</td>
<td>0,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>2 a 4'm2'</td>
<td>0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_o, 4mm
\(a^* = (a - b)/2 \quad b^* = (a + b)/2\):
Along [1,0,0] p2mg1'
\(a^* = b \quad b^* = c\):
Along [1,1,0] p2mm'
\(a^* = -c/2 \quad b^* = (-a + b)/2\):
Origin at 0,0,z
Origin at x,1/4,1/4
Origin at x,x,0
Origin at $\overline{4}m'2'n$, at $-1/4,1/4,-1/4$ from $\overline{1}'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(1) $0,0,0$

(5) 2 (0.1,2,0) $1/4,y,1/4$
(2, $1/2,1/2,1/2$

(9) $\overline{1} 1/4,1/4,1/4$
(1 $1/2,1/2,1/2'$

(13) m $x,0,z$
(m $0,0,0'$

(2) 2 0,0,z
(2 $z,0,0,0$

(6) 2 (1/2,0,0) $x,1/4,1/4$
(2 $x,1/2,1/2,1/2$

(10) n' (1/2,1/2,0) $x,y,1/4$
(m $1/2,1/2,1/2'$

(14) m' $0,y,z$
(m $0,0,0'$

(3) $4' \cdot (0,0,1/2) 0,1/2,z$
($4',1/2,1/2,1/2'$

(4) $4' \cdot (0,0,1/2) 1/2,0,z$
($4',1/2,1/2,1/2'$

(7) 2' $x,x,0$
($2',0,0,0$

(8) 2' $x,x,0$
($2',0,0,0'$

(11) $\overline{4} \cdot 0,0,z; 0,0,0$
($\overline{4},0,0,0$

(12) $\overline{4} \cdot 0,0,z; 0,0,0$
($\overline{4},0,0,0'$

(15) c (0.0,1/2) $x+1/2,x,z$
(m $1/2,1/2,1/2$

(16) n (1/2,1/2,1/2) $x,x,z$
(m $1/2,1/2,1/2$

P4$_2'/n'm'c$

137.6.1166

$4'/m'm'm$

P4$_2'/n'm'2'/c$

137.6.1166 - 1 - 2452
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
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<td>8 g .m'. 0,y,z [0,v,w]</td>
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<td>1/4,3/4,1/4 [0,0,0]</td>
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<tr>
<td>4 d 2m'm'. 0,1/2,z [0,0,w]</td>
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<td>1/2,0,z+1/2 [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<tr>
<td>2 b 4m'2' 0,0,1/2 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
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<td>2 a 4m'2' 0,0,0 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p4' mm'  
  \( \mathbf{a}' = (\mathbf{a} - \mathbf{b})/2 \)  
  \( \mathbf{b}' = (\mathbf{a} + \mathbf{b})/2 \)  
  Origin at 0,0,z

- Along [1,0,0] p2m'g'  
  \( \mathbf{a}' = \mathbf{b} \)  
  \( \mathbf{b}' = \mathbf{c} \)  
  Origin at x,1/4,1/4

- Along [1,1,0] p_{2a} 2m'm'  
  \( \mathbf{a}' = -c/2 \)  
  \( \mathbf{b}' = -(\mathbf{a} + \mathbf{b})/2 \)  
  Origin at x,x,0
**Origin** at $\bar{4}m'2'/n'$, at $-1/4,1/4,-1/4$ from $\bar{1}$

**Asymmetric unit**

$0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/4$

**Symmetry Operations**

(1) 1

(1) $\bar{1}$

(5) $2' (0,1/2,0) \quad 1/4,y,1/4$

(2) $2' (1/2,0,0) \quad x,1/4,1/4$

(2) $2' (1/2,0,0) \quad x,1/4,1/4$

(9) $\bar{1} 1/4,1/4,1/4$

(10) $n (1/2,1/2,0) \quad x,y,1/4$

(10) $n (1/2,1/2,0) \quad x,y,1/4$

(13) $m' \quad x,0,z$

(14) $m' \quad 0,y,z$

(15) $c' (0,0,1/2) \quad x+1/2,x,z$

(16) $n' (1/2,1/2,1/2) \quad x,x,z$

(1) 1

(1) $\bar{1}$

(5) $2' (0,1/2,0) \quad 1/4,y,1/4$

(2) $2' (1/2,0,0) \quad x,1/4,1/4$

(2) $2' (1/2,0,0) \quad x,1/4,1/4$

(9) $\bar{1} 1/4,1/4,1/4$

(10) $n (1/2,1/2,0) \quad x,y,1/4$

(10) $n (1/2,1/2,0) \quad x,y,1/4$

(13) $m' \quad x,0,z$

(14) $m' \quad 0,y,z$

(15) $c' (0,0,1/2) \quad x+1/2,x,z$

(16) $n' (1/2,1/2,1/2) \quad x,x,z$
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

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8 g .m'.  | 0, y, z [0, v, w] | 0, y, z [0, v, w] | y + 1/2, 1/2, z + 1/2 [v, 0, w] | y + 1/2, 1/2, z + 1/2 [v, 0, w] |
|           | 1/2, y + 1/2, z + 1/2 [0, v, w] | 1/2, y + 1/2, z + 1/2 [0, v, w] | y, 0, z [v, 0, w] | y, 0, z [v, 0, w] |

8 f .2'   | x, x, 0 [u, u, w] | x, x, 0 [u, u, w] | x + 1/2, x + 1/2, 1/2 [u, u, w] | x + 1/2, x + 1/2, 1/2 [u, u, w] |
|           | x + 1/2, x + 1/2, 1/2 [u, u, w] | x + 1/2, x + 1/2, 1/2 [u, u, w] | x, x, 0 [u, u, w] | x, x, 0 [u, u, w] |


4 d 2m' m' | 0, 1/2, z [0, 0, w] | 0, 1/2, z + 1/2 [0, 0, w] | 1/2, 0, z + 1/2 [0, 0, w] | 1/2, 0, z [0, 0, w] |

4 c 2m' m' | 0, 0, z [0, 0, w] | 1/2, 1/2, z + 1/2 [0, 0, w] | 1/2, 1/2, z + 1/2 [0, 0, w] | 0, 0, z [0, 0, w] |

2 b 4m' 2'  | 0, 0, 1/2 [0, 0, w] | 1/2, 1/2, 0 [0, 0, w] | 1/2, 1/2, 0 [0, 0, w] | 0, 0, z [0, 0, w] |

2 a 4m' 2'  | 0, 0, 0 [0, 0, w] | 1/2, 1/2, 1/2 [0, 0, w] | 1/2, 1/2, 1/2 [0, 0, w] | 0, 0, z [0, 0, w] |

**Symmetry of Special Projections**

Along [0,0,1] p_c 4m' m'

\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]

Origin at 0, 1/2, z

Along [1,0,0] p2'm' g

\[ \mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c} \]

Origin at x, 1/4, 1/4

Along [1,1,0] p2' mm' g

\[ \mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]

Origin at x, x, 0
**Origin** at $\bar{4}m2/n'$, at $-1/4,1/4,-1/4$ from $\bar{1}'$.

**Asymmetric unit**

$0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/4$

**Symmetry Operations**

1. $1$
   
   Origin

2. $2' (0,0,0)$
   
   $x,0,0$ (2 $z,0,0$)

3. $4' (0,0,1/2) 0,1/2,z$
   
   $4 (z_1,1/2,1,1/2')$ ($2,0,0$)

4. $4' (0,0,1/2) 1/2,0,z$
   
   $4 (1/2,1/2,1/2')$ ($2,1/2,1/2')$

5. $2' (1/2,0,0) x,1/4,1/4$
   
   $2 (2,1/2,1/2')$

6. $2' (1/2,0,0) x,1/4,1/4$
   
   $2 (2,1/2,1/2')$

7. $x,x,0$
   
   $2 (2,0,0)$

8. $x,x,0$
   
   $2 (2,0,0)$

9. $1/4,1/4,1/4$
   
   $1/4,1/4,1/4$

10. $1/2,1/2,1/2'$
    
   $1/2,1/2,1/2'$

11. $0,0,0$
    
   $0,0,0$

12. $0,0,0$
    
   $0,0,0$

13. $x,0,z$
    
   $2 (m,0,0)$

14. $0,y,z$
    
   $2 (m,0,0)$

15. $0,0,1/2$ x+1/2, x, z
    
   $0,0,1/2$ x+1/2, x, z

16. $1/2,1/2,1/2$
    
   $1/2,1/2,1/2'$

**137.8.1168 - 1 - 2456**
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

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<td>(9) y + 1/2, x + 1/2, z + 1/2 [v, u, w] (10) x + 1/2, y + 1/2, z + 1/2 [u, v, w]</td>
</tr>
<tr>
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<td>(11) y, x, z [v, u, w] (12) y, x, z [v, u, w]</td>
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<tr>
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<td>(13) x, y, z [u, v, w] (14) x, y, z [u, v, w]</td>
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<td>(15) y + 1/2, x + 1/2, z + 1/2 [v, u, w] (16) y + 1/2, x + 1/2, z + 1/2 [v, u, w]</td>
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<tr>
<td>2 b 4mm</td>
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<td>2 a 4mm</td>
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</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1] p4'm'm
along [1,0,0] p2mg1'
along [1,1,0] p2'2mm'
a* = (a - b)/2 b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] p2mg1'
a* = b b* = c
Origin at x,1/4,1/4

Along [1,1,0] p2'2mm'
a* = -c/2 b* = (-a + b)/2
Origin at x,x,0
Origin at $\overline{4}m'2/n'$, at $-1/4,1/4,-1/4$ from $1'$

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4$

Symmetry Operations

(1) 1
(1') 0,0,0

(2) 2 0,0,z
(2_z) 0,0,0

(3) $4^+$ (0,0,1/2) 0,1/2,z
(4_z) 1/2,1/2,1/2

(4) $4^-$ (0,0,1/2) 1/2,0,z
(4_z^-1) 1/2,1/2,1/2

(5) 2 (0,1/2,0) 1/4,y,1/4
(2_y) 1/2,1/2,1/2

(6) 2 (1/2,0,0) x,1/4,1/4
(2_x) 1/2,1/2,1/2

(7) 2 x,x,0
(2_x) 0,0,0

(8) 2 x,x,0
(2_x) 0,0,0

(9) $\overline{1}$ 1/4,1/4,1/4
(1') 1/2,1/2,1/2

(10) $n'$ (1/2,1/2,0) x,y,1/4
(m_z) 1/2,1/2,1/2

(11) $\overline{4}^+$ 0,0,z; 0,0,0
(4_z) 0,0,0

(12) $\overline{4}^-$ 0,0,z; 0,0,0
(4_z^-1) 0,0,0

(13) $m'$ x,0,z
(m_z) 0,0,0

(14) $m'$ 0,y,z
(m_y) 0,0,0

(15) $c'$ (0,0,1/2) x+1/2,z
(m_{xy}) 1/2,1/2,1/2

(16) $n'$ (1/2,1/2,1/2) x,x,z
(m_{xy}) 1/2,1/2,1/2
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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<th>Number</th>
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<th>Position</th>
<th>Coordinate</th>
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<tr>
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<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
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<td>0,y, z [0,v,w]</td>
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<tr>
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<td>0,1/2, z [0,0,w]</td>
<td>0,1/2, z + 1/2 [0,0,w]</td>
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<td>1/2, 0, z + 1/2 [0,0,w]</td>
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<td>1/2, 1/2, z + 1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>0,0, 1/2 [0,0,0]</td>
<td>1/2, 1/2, 0 [0,0,0]</td>
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<tr>
<td>2</td>
<td>a</td>
<td>0,0, 0 [0,0,0]</td>
<td>1/2, 1/2, 1/2 [0,0,0]</td>
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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4m’m’</th>
<th>Along [1,0,0] p2m’g’</th>
<th>Along [1,1,0] p2m’m’</th>
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<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>a* = b</td>
<td>a* = (-a + b)/2</td>
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<tr>
<td>b* = (a + b)/2</td>
<td>b* = c</td>
<td>b* = c/2</td>
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</tbody>
</table>

Origin at 0,0,z
Origin at x,1/4,1/4
Origin at x,x,0
**Origin** at $\overline{4}cg$, at $-1/4,1/4,-1/4$ from center (2/m)

**Asymmetric unit**

\[
0 \leq x < 1/4; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1; \quad x < y; \quad y < 1/2 - x
\]

**Symmetry Operations**

1. $1$
   
2. $2 \cdot 0,0,z$
   
3. $4^+ (0,0,1/2) 0,1/2,z$
   
4. $4^- (0,0,1/2) 1/2,0,z$
   
5. $2 \cdot (0,1/2,0) 1/4,y,0$
   
6. $2 \cdot (1/2,0,0) x,1/4,0$
   
7. $2 \cdot x,x,1/4$
   
8. $2 \cdot x,x,1/4$
   
9. $\overline{1} \cdot 1/4,1/4,1/4$
   
10. $n \cdot (1/2,1/2,0) x,y,1/4$
    
11. $\overline{4}^+ 0,0,z; 0,0,0$
    
12. $\overline{4}^- 0,0,z; 0,0,0$
    
13. $c \cdot (0,0,1/2) x,0,z$
    
14. $c \cdot (0,0,1/2) 0,y,z$
    
15. $m \cdot x+1/2,x,z$
    
16. $g \cdot (1/2,1/2,0) x,x,z$

---

**P4$_2$/nmc**

**4/mmm**

**Tetragonal**

**138.1.1170**
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<tbody>
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<td>16</td>
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<td>(1) x,y,z [u,v,w]</td>
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<td>(4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(7) y,x̅+1/2,x+1/2,z+1/2 [v,u̅,w̅]</td>
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<td>..m</td>
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<td>..2/m</td>
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<tr>
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<td>..2/m</td>
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</table>

138.1.1170 - 2 - 2461
Symmetry of Special Projections

Along [0,0,1]  \( p_{4m} \) 4mm  
\[ a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \]  
Origin at 0,0,z

Along [1,0,0]  \( p_{2m1} \) 2m'g'  
\[ a^* = b \quad b^* = \frac{c}{2} \]  
Origin at x,1/4,0

Along [1,1,0]  \( p_{2mm1} \)  
\[ a^* = \frac{-a + b}{2} \quad b^* = c \]  
Origin at x,x,1/4
**Origin** at \( \overline{4} \)c1', at \(-1/4,1/4,-1/4\) from center (2/m1')

**Asymmetric unit**

\[
0 < x < 1/4; \quad 0 < y < 1/2; \quad 0 < z < 1; \quad x < y; \quad y < 1/2 - x
\]

**Symmetry Operations**

For 1 + set

1. \[(1) \quad 1 \quad (1|0,0,0)\]
2. \[(2) \quad 2 \quad 0,0,z \quad (2z|0,0,0)\]
3. \[(3) \quad 4^+ \quad (0,0,1/2) \quad 0,1/2,z \quad (4_z|1/2,1/2,1/2)\]
4. \[(4) \quad 4^- \quad (0,0,1/2) \quad 1/2,0,z \quad (4_z^-|1/2,1/2,1/2)\]
5. \[(5) \quad 2 \quad (0,1/2,0) \quad 1/4,y,0 \quad (2_y|1/2,1/2,0)\]
6. \[(6) \quad 2 \quad (1/2,0,0) \quad x,1/4,0 \quad (2_x|1/2,1/2,0)\]
7. \[(7) \quad 2 \quad x,x,1/4 \quad (2_{xy}|0,0,1/2)\]
8. \[(8) \quad 2 \quad x,x,1/4 \quad (2_{xy}|0,0,1/2)\]
9. \[(9) \quad \overline{1} \quad 1/4,1/4,1/4 \quad (1\overline{1}|1/2,1/2,1/2)\]
10. \[(10) \quad n \quad (1/2,1/2,0) \quad x,y,1/4 \quad (m_z|1/2,1/2,1/2)\]
11. \[(11) \quad 4^+ \quad 0,0,z; \quad 0,0,0 \quad (4_z|0,0,0)\]
12. \[(12) \quad 4^- \quad 0,0,z; \quad 0,0,0 \quad (4_z^-|0,0,0)\]
13. \[(13) \quad c \quad (0,0,1/2) \quad x,0,z \quad (m|0,0,1/2)\]
14. \[(14) \quad c \quad (0,0,1/2) \quad 0,y,z \quad (m_y|0,0,1/2)\]
15. \[(15) \quad m \quad x+1/2,\overline{x},z \quad (4_{xy}|1/2,1/2,0)\]
16. \[(16) \quad g \quad (1/2,1/2,0) \quad x,x,z \quad (m_{xy}|1/2,1/2,0)\]
For 1' + set

<table>
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<th>Coordinates</th>
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<td>(2) x,y,z [0,0,0]</td>
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</table>

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9); 1'.

Positions

Multiplicity
Wyckoff letter
Site Symmetry

1 +

16 j 11'

(1) x,y,z [0,0,0]
(2) x,y,z [0,0,0]
(3) y+1/2,x+1/2,z+1/2 [0,0,0]
(4) y+1/2,x+1/2,z+1/2 [0,0,0]
(5) x+1/2,y+1/2,z [0,0,0]
(6) x+1/2,y+1/2,z [0,0,0]
(7) y,x,z+1/2 [0,0,0]
(8) y,x,z+1/2 [0,0,0]
(9) x+1/2,y+1/2,z+1/2 [0,0,0]
(10) x+1/2,y+1/2,z+1/2 [0,0,0]
(11) y,x,z [0,0,0]
(12) y,x,z [0,0,0]
(13) x,y,z+1/2 [0,0,0]
(14) x,y,z+1/2 [0,0,0]
(15) y+1/2,x+1/2,z [0,0,0]
(16) y+1/2,x+1/2,z [0,0,0]
<p>| | | | | | | | |</p>
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<td>d</td>
<td>.2/m1'</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,1/4 [0,0,0]</td>
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<tr>
<td>4</td>
<td>c</td>
<td>.2/m1'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>1/4,3/4,3/4 [0,0,0]</td>
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<td></td>
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<tr>
<td>4</td>
<td>b</td>
<td>4..1'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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</tr>
<tr>
<td>4</td>
<td>a</td>
<td>2.221'</td>
<td>0,0,1/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
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</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'

- $a^* = (a - b)/2$
- $b^* = (a + b)/2$

Origin at 0,0,z

Along [1,0,0] p2mg1'

- $a^* = b$
- $b^* = c/2$

Origin at x,1/4,0

Along [1,1,0] p2mm1'

- $a^* = (-a + b)/2$
- $b^* = c$

Origin at x,x,1/4
Origin at $4\bar{4}cg$, at $-1/4,1/4,-1/4$ from center (2/m)

Asymmetric unit

$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y; \quad y \leq 1/2 - x$

Symmetry Operations

(1) 1
(1 0 0)

(5) 2 (0,1/2,0) 1/4,y,0
(2$x$ | 1/2,1/2,0)

(9) $\bar{1}$ 1/4,1/4,1/4
(1 1/2,1/2,1/2)

(13) c (0,0,1/2) x,0,z
(m$y$ | 0,0,1/2)

(2) 2 0,0,z
(2$x$ | 0,0,0)

(6) 2' (1/2,0,0) x,1/4,0
(2$x$ | 1/2,1/2,0)

(10) n' (1/2,1/2,0) x,y,1/4
(m$z$ | 1/2,1/2,1/2)

(3) 4' (0,0,1/2) 0,1/2,z
(4$x$ | 1/2,1/2,1/2)

(7) 2' x,x,1/4
(2$y$ | 0,1/2)

(11) $\bar{4}'$ 0,0,z; 0,0,0
(4$x$ | 0,0,0)

(14) c (0,0,1/2) 0,y,z
(m$z$ | 0,0,1/2)

(4) 4' (0,0,1/2) 1/2,0,z
(4$x$ | 1/2,1/2,1/2)

(8) 2' x,x,1/4
(2$y$ | 0,0,1/2)

(15) m x+1/2,x,z
(m$y$ | 1/2,1/2,0)

(12) $\bar{4}'$ 0,0,z; 0,0,0
(4$x$ | 0,0,0)

(16) g (1/2,1/2,0) x,x,z
(m$y$ | 1/2,1/2,0)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

16 j 1

(1) x,y,z [u,v,w]  
(2) x,y,z [u,v,w]  
(3) y+1/2,x+1/2,z+1/2 [v,u,w]  
(4) y+1/2,x+1/2,z+1/2 [v,u,w]  
(5) x+1/2,y+1/2,z [u,v,w]  
(6) x+1/2,y+1/2,z [u,v,w]  
(7) x+1/2,y+1/2,z+1/2 [v,u,w]  
(8) x+1/2,y+1/2,z+1/2 [v,u,w]  
(9) x+1/2,y+1/2,z+1/2 [u,v,w]  
(10) x+1/2,y+1/2,z+1/2 [u,v,w]  
(11) y,x,z [v,u,w]  
(12) y,x,z [v,u,w]  
(13) y,x,z [v,u,w]  
(14) y,x,z [v,u,w]  
(15) y+1/2,x+1/2,z [v,u,w]  
(16) y+1/2,x+1/2,z [v,u,w]  

8 i ..m

x,x+1/2,z [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  
(1/2,1/2,z+1/2 [u,u,0]  

8 h ..2'

x,x,3/4 [u,u,w]  
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(1/2,1/2,3/4 [u,u,w]  
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(1/2,1/2,3/4 [u,u,w]  
(1/2,1/2,3/4 [u,u,w]  

8 g ..2'

x,x,1/4 [u,u,w]  
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(1/2,1/2,3/4 [u,u,w]  
(1/2,1/2,3/4 [u,u,w]  
(1/2,1/2,3/4 [u,u,w]  

8 f ..2

0,0,z [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
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(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  

4 e 2.mm

0,1/2,z [0,0,0]  
(1/2,0,z+1/2 [0,0,0]  
(1/2,0,z+1/2 [0,0,0]  
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(1/2,0,z+1/2 [0,0,0]  
(1/2,0,z+1/2 [0,0,0]  
(1/2,0,z+1/2 [0,0,0]  
(1/2,0,z+1/2 [0,0,0]  

4 d ..2'm

1/4,1/4,3/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
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(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  

4 c ..2'm

1/4,1/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  
(3/4,3/4,1/4 [0,0,0]  

4 b 4'..

0,0,0 [0,0,0]  
(1/2,1/2,1/2 [0,0,0]  
(1/2,1/2,1/2 [0,0,0]  
(1/2,1/2,1/2 [0,0,0]  
(1/2,1/2,1/2 [0,0,0]  
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(1/2,1/2,1/2 [0,0,0]  
(1/2,1/2,1/2 [0,0,0]  

4 a 2.2'2

0,0,1/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  
(1/2,1/2,3/4 [0,0,w]  

Continued 138.3.1172 P4₂/n'cm
Continued

Symmetry of Special Projections

Along [0,0,1] p4mm
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] \( p_{2b} \) 2m'g'
\[ a^* = b \quad b^* = c/2 \]
Origin at x,1/4,1/4

Along [1,1,0] p2mm1'
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,1/4
Origin at $\bar{4}c'g$, at $-1/4,1/4,-1/4$ from center (2/m)

Symmetry Operations

(1) 1
(1, 0, 0, 0)

(2) $2', 0,0,z$
(2, 0, 0, 0)

(3) $4^+ \cdot (0,0,1/2), 0,1/2,z$
(4, 1/2, 1, 1/2, 1/2, 1/2)'

(4) $4^- \cdot (0,0,1/2), 1/2,0,z$
(4, 1/2, 1/2, 1/2, 1/2)'

(5) $2' (0,1/2,0)$

(6) $2' (1/2,0,0)$

(7) $2$x, x, 1/4
(2, x, 0, 1/2)

(8) $2$ x, x, 1/4
(2, x, 0, 1/2)

(9) $\bar{1} 1/4,1/4,1/4$

(10) n (1/2, 1/2, 0)

(11) $\bar{4}^- \cdot 0,0,z; 0,0,0$

(12) $\bar{4}^- \cdot 0,0,z; 0,0,0$

(13) $c' (0,0,1/2)$

(14) $c' (0,0,1/2)$

(15) m x+1/2, x, z

(16) g (1/2, 1/2, 0)

Asymmetric unit

$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y; \quad y \leq 1/2 - x$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

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<th>Coordinates</th>
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<td>16 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(8) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>8 i ..m</td>
<td>(9) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(10) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(16) y+1/2,x+1/2,z [v,u,w]</td>
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<td>x,x+1/2,z [u,u,0]</td>
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<td>x,x+1/2,z [u,u,0]</td>
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<td>x+1/2,x,z [u,u,0]</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] p_{\infty} 4mm
\( a^* = \frac{a - b}{2} \quad b^* = \frac{a + b}{2} \)
Origin at 0,0,z

Along [1,0,0] p2m'g
\( a^* = b \quad b^* = \frac{c}{2} \)
Origin at x,1/4,0

Along [1,1,0] p2mm1'
\( a^* = \frac{-a + b}{2} \quad b^* = c \)
Origin at x,x,1/4
Origin at \( \overline{4}c'g \), at \(-1/4, 1/4, -1/4\) from center (\(2'm'\))

Asymmetric unit  
\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x < y; \quad y < 1/2 - x \]

Symmetry Operations

1. \(1\)  
   \( (1|0,0,0) \)

2. \(2\)  
   \( (0,0,z) \)  
   \( (2_z|0,0,0) \)

3. \(4^+\)  
   \( (0,0,1/2) \)  
   \( (0,1/2,z) \)  
   \( (4_z|1/2,1/2,1/2') \)

4. \(4^-\)  
   \( (0,0,1/2) \)  
   \( (1/2,0,z) \)  
   \( (4_z|1/2,1/2,1/2') \)

5. \(2\)  
   \( (0,1/2,0) \)  
   \( (1/2,1,2,0) \)

6. \(2\)  
   \( (1,2,0,0) \)  
   \( (1,2,1,2,0) \)

7. \(2\)  
   \( (x,x,1/4) \)  
   \( (2_{xy}|0,0,1/2') \)

8. \(2\)  
   \( (x,x,1/4) \)  
   \( (2_{xy}|0,0,1/2') \)

9. \(\overline{1}\)  
   \( 1/4,1/4,1/4 \)  
   \( (1|1/2,1/2,1/2) \)

10. \(n\)  
    \( (1/2,1/2,0) \)  
    \( (x,y,1/4) \)  
    \( (m_z|1/2,1/2,1/2) \)

11. \(\overline{4}^+\)  
    \( (0,0,0) \)  
    \( (0,0,0) \)  
    \( (4_z|0,0,0') \)

12. \(\overline{4}^-\)  
    \( (0,0,0) \)  
    \( (0,0,0) \)  
    \( (4_z|0,0,0') \)

13. \(c\)  
    \( (0,0,1/2) \)  
    \( x,0,z \)  
    \( (m_j|0,0,1/2) \)

14. \(c\)  
    \( (0,0,1/2) \)  
    \( 0,y,z \)  
    \( (m_j|0,0,1/2) \)

15. \(m'\)  
    \( x+1/2, x, z \)  
    \( (m_{xy}|1/2,1/2,0) \)

16. \(g'\)  
    \( (1/2,1/2,0) \)  
    \( x,x,z \)  
    \( (m_{xy}|1/2,1/2,0) \)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

**Positions**

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
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<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>(11) y,x,z [v,u,w]</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>$a^*$</th>
<th>$b^*$</th>
<th>Origin</th>
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</thead>
<tbody>
<tr>
<td>$[0,0,1]$</td>
<td>$p_{4mm}$</td>
<td>$(a - b)/2$</td>
<td>$(a + b)/2$</td>
<td>0,0,z</td>
</tr>
<tr>
<td>$[1,0,0]$</td>
<td>$p_{2m'}$</td>
<td>$b$</td>
<td>$c/2$</td>
<td>x,1/4,0</td>
</tr>
<tr>
<td>$[1,1,0]$</td>
<td>$p_{2mm'}$</td>
<td>$-c$</td>
<td>$(-a + b)/2$</td>
<td>x,x,1/4</td>
</tr>
</tbody>
</table>
**Origin** at $\overline{4}c'g$, at $-1/4,1/4,-1/4$ from center $2'm$)

**Asymmetric unit**

\begin{align*}
0 \leq x & \leq 1/4; & 0 \leq y & \leq 1/2; & 0 \leq z & \leq 1; & x < y; & y \leq 1/2 - x
\end{align*}

**Symmetry Operations**

\begin{align*}
(1) & \ 1 \quad (1 \ | \ 0,0,0) \\
(2) & \ 2 \ 0,0,z \quad (2_z \ | \ 0,0,0) \\
(3) & \ 4\times' \ (0,0,1/2) \ 0,1/2,z \quad (4_z \ | \ 1/2,1/2,1/2') \\
(4) & \ 4\times' \ (0,0,1/2) \ 1/2,0,z \quad (4_z \ | \ 1/2,1/2,1/2') \\
(5) & \ 2 \ (0,1/2,0) \ 1/4,y,0 \quad (2_y \ | \ 1/2,1/2,0) \\
(6) & \ 2 \ (1/2,0,0) \ x,1/4,0 \quad (2_x \ | \ 1/2,1/2,0) \\
(7) & \ 2' \ x,x,1/4 \quad (2_{xy} \ | \ 0,0,1/2') \\
(8) & \ 2' \ x,x,1/4 \quad (2_{xy} \ | \ 0,0,1/2') \\
(9) & \ \overline{1} \ 1/4,1/4,1/4 \quad (1 \ | \ 1/2,1/2,1/2') \\
(10) & \ n' \ (1/2,1/2,0) \ x,y,1/4 \quad (m_x \ | \ 1/2,1/2,1/2') \\
(11) & \ 4\times' \ 0,0,z; \ 0,0,0 \quad (4_z \ | \ 0,0,0) \\
(12) & \ \overline{4}\times \ 0,0,z; \ 0,0,0 \quad (4_{yz} \ | \ 0,0,0) \\
(13) & \ c' \ (0,0,1/2) \ x,0,z \quad (m_y \ | \ 0,0,1/2') \\
(14) & \ c' \ (0,0,1/2) \ 0,y,z \quad (m_y \ | \ 0,0,1/2') \\
(15) & \ m \ x+1/2,x,z \quad (m_{yx} \ | \ 1/2,1/2,0) \\
(16) & \ g \ (1/2,1/2,0) \ x,x,z \quad (m_{yx} \ | \ 1/2,1/2,0)
\end{align*}
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
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<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
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<td>(4) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
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<td>(7) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
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<td>(8) y,x,z+1/2 [v,u,w]</td>
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<td>(9) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
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<td>(10) x+1/2,y+1/2,z+1/2 [v,u,w]</td>
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(11) y,x,z [v, u, w]

(12) y,x,z [v, u, w]

(13) x,y,z+1/2 [u, v, w]

(14) x,y+1/2 [u, v, w]

(15) x+1/2,x+1/2,z [v, u, w]

(16) x+1/2,x+1/2,z [v, u, w]

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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Formula 1</th>
<th>Formula 2</th>
<th>Formula 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4'mm'</td>
<td>(a^* = (a - b)/2)</td>
<td>(b^* = (a + b)/2)</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p 2m'g'</td>
<td>(a^* = b)</td>
<td>(b^* = c/2)</td>
<td>Origin at 1/4,0</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p2mm1'</td>
<td>(a^* = (-a + b)/2)</td>
<td>(b^* = c)</td>
<td>Origin at x,x,1/4</td>
</tr>
</tbody>
</table>
**Origin** at $\bar{4}c'g'$, at $-1/4,1/4,-1/4$ from center (2'/m')

**Asymmetric unit**

$0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x < y; \quad y \leq 1/2 - x$

**Symmetry Operations**

1. $1$

2. $2 \quad 0,0,z$

3. $4^+ (0,0,1/2) \quad 0,1/2,z$

4. $4^- (0,0,1/2) \quad 1/2,0,z$

5. $2' (0,1/2,0) \quad 1/4,y,0$

6. $2' (1/2,0,0) \quad x,1/4,0$

7. $2' x, x, 1/4$

8. $2' x, x, 1/4$

9. $\bar{1} 1/4,1/4,1/4$

10. $n (1/2,1/2,0) \quad x,y,1/4$

11. $\bar{4}^+ 0,0,z; \quad 0,0,0$

12. $\bar{4}^- 0,0,z; \quad 0,0,0$

13. $c' (0,0,1/2) \quad x,0,z$

14. $c' (0,0,1/2) \quad 0,y,z$

15. $m' x+1/2, x,z$

16. $g' (1/2,1/2,0) \quad x,x,z$

---

138.7.1176 - 1 - 2478
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tr>
<td>16 j 1</td>
<td>1</td>
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| 8 i .m'      | 8              | (1) x+1/2,z [u,u,w] |
|              |                | (2) x+1/2,z [u,u,w] |
|              |                | (3) x+1/2,z [u,u,w] |
|              |                | (4) x+1/2,z [u,u,w] |
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|              |                | (11) x+1/2,z [u,u,w] |
|              |                | (12) x+1/2,z [u,u,w] |

| 8 h .2'      | 8              | (1) x+1/2,z [u,u,w] |
|              |                | (2) x+1/2,z [u,u,w] |
|              |                | (3) x+1/2,z [u,u,w] |
|              |                | (4) x+1/2,z [u,u,w] |
|              |                | (5) x+1/2,z [u,u,w] |
|              |                | (6) x+1/2,z [u,u,w] |
|              |                | (7) x+1/2,z [u,u,w] |
|              |                | (8) x+1/2,z [u,u,w] |

| 8 g .2'      | 8              | (1) x+1/2,z [u,u,w] |
|              |                | (2) x+1/2,z [u,u,w] |
|              |                | (3) x+1/2,z [u,u,w] |
|              |                | (4) x+1/2,z [u,u,w] |
|              |                | (5) x+1/2,z [u,u,w] |
|              |                | (6) x+1/2,z [u,u,w] |
|              |                | (7) x+1/2,z [u,u,w] |
|              |                | (8) x+1/2,z [u,u,w] |

| 8 f 2..      | 8              | (1) 0,0,z [0,0,w] |
|              |                | (2) 0,0,z [0,0,w] |
|              |                | (3) 0,0,z [0,0,w] |
|              |                | (4) 0,0,z [0,0,w] |
|              |                | (5) 0,0,z [0,0,w] |
|              |                | (6) 0,0,z [0,0,w] |
|              |                | (7) 0,0,z [0,0,w] |
|              |                | (8) 0,0,z [0,0,w] |

| 4 e 2.m'     | 4              | (1) 0,1/2,z [0,0,w] |
|              |                | (2) 0,1/2,z [0,0,w] |
|              |                | (3) 0,1/2,z [0,0,w] |
|              |                | (4) 0,1/2,z [0,0,w] |
|              |                | (5) 0,1/2,z [0,0,w] |
|              |                | (6) 0,1/2,z [0,0,w] |
|              |                | (7) 0,1/2,z [0,0,w] |
|              |                | (8) 0,1/2,z [0,0,w] |

| 4 d .2'/m'   | 4              | (1) 1/4,1/4,3/4 [u,u,w] |
|              |                | (2) 1/4,1/4,3/4 [u,u,w] |
|              |                | (3) 1/4,1/4,3/4 [u,u,w] |
|              |                | (4) 1/4,1/4,3/4 [u,u,w] |
|              |                | (5) 1/4,1/4,3/4 [u,u,w] |
|              |                | (6) 1/4,1/4,3/4 [u,u,w] |
|              |                | (7) 1/4,1/4,3/4 [u,u,w] |
|              |                | (8) 1/4,1/4,3/4 [u,u,w] |

| 4 c .2'/m'   | 4              | (1) 1/4,1/4,1/4 [u,u,w] |
|              |                | (2) 1/4,1/4,1/4 [u,u,w] |
|              |                | (3) 1/4,1/4,1/4 [u,u,w] |
|              |                | (4) 1/4,1/4,1/4 [u,u,w] |
|              |                | (5) 1/4,1/4,1/4 [u,u,w] |
|              |                | (6) 1/4,1/4,1/4 [u,u,w] |
|              |                | (7) 1/4,1/4,1/4 [u,u,w] |
|              |                | (8) 1/4,1/4,1/4 [u,u,w] |

| 4 b 4..      | 4              | (1) 0,0,0 [0,0,w] |
|              |                | (2) 0,0,0 [0,0,w] |
|              |                | (3) 0,0,0 [0,0,w] |
|              |                | (4) 0,0,0 [0,0,w] |
|              |                | (5) 0,0,0 [0,0,w] |
|              |                | (6) 0,0,0 [0,0,w] |
|              |                | (7) 0,0,0 [0,0,w] |
|              |                | (8) 0,0,0 [0,0,w] |

| 4 a 2.2'     | 4              | (1) 0,0,1/4 [0,0,w] |
|              |                | (2) 0,0,1/4 [0,0,w] |
|              |                | (3) 0,0,1/4 [0,0,w] |
|              |                | (4) 0,0,1/4 [0,0,w] |
|              |                | (5) 0,0,1/4 [0,0,w] |
|              |                | (6) 0,0,1/4 [0,0,w] |
|              |                | (7) 0,0,1/4 [0,0,w] |
|              |                | (8) 0,0,1/4 [0,0,w] |
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4, 4m'</td>
<td>a* = (a - b)/2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>b* = (a + b)/2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2mg</td>
<td>a* = b</td>
</tr>
<tr>
<td></td>
<td></td>
<td>b* = c/2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Origin at x,1/4,0</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p2'mm'</td>
<td>a* = -c</td>
</tr>
<tr>
<td></td>
<td></td>
<td>b* = (-a + b)/2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Origin at x,x,1/4</td>
</tr>
</tbody>
</table>

**Explanation:**
- \( a^* = \frac{a - b}{2} \)
- \( b^* = \frac{a + b}{2} \)
- \( a^* = b \)
- \( b^* = \frac{c}{2} \)
- \( a^* = -c \)
- \( b^* = \frac{-a + b}{2} \)
Origin at $\overline{4}cg'$, at $-1/4,1/4,-1/4$ from center (2/m')

Asymmetric unit $0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq y; \quad y \leq 1/2 - x$

Symmetry Operations

1. $1$
   
2. $2 \cdot \begin{pmatrix} 0,0,0 \end{pmatrix}$
   
3. $4^{+} \cdot \begin{pmatrix} 0,0,1/2 \end{pmatrix}$
4. $4^{-} \cdot \begin{pmatrix} 0,0,1/2 \end{pmatrix}$

5. $2' \cdot \begin{pmatrix} 0,1/2,0 \end{pmatrix}$
6. $2' \cdot \begin{pmatrix} 1/2,0,0 \end{pmatrix}$
7. $2 \cdot \begin{pmatrix} x,x,1/4 \end{pmatrix}$
8. $2 \cdot \begin{pmatrix} x,y,1/4 \end{pmatrix}$

9. $\overline{1} \cdot \begin{pmatrix} 1/4,1/4,1/4 \end{pmatrix}$
10. $\overline{1} \cdot \begin{pmatrix} 1/2,1/2,1/2 \end{pmatrix}$
11. $\overline{4}^{-} \cdot \begin{pmatrix} 0,0,0 \end{pmatrix}$
12. $\overline{4}^{+} \cdot \begin{pmatrix} 0,0,0 \end{pmatrix}$

13. $c \cdot \begin{pmatrix} 0,0,1/2 \end{pmatrix}$
14. $c \cdot \begin{pmatrix} 0,0,1/2 \end{pmatrix}$
15. $m' \cdot \begin{pmatrix} x+1/2,y,z \end{pmatrix}$
16. $g' \cdot \begin{pmatrix} 1/2,1/2,0 \end{pmatrix}$
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

### Positions
Multplicity,  
Wyckoff letter,  
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<td>(2) x,y,z [u,v,w]</td>
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<td>(3) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(15) y+1/2,x+1/2,z [v,u,w]</td>
<td>(16) y+1/2,x+1/2,z [v,u,w]</td>
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<td>x,x+1/2,z [u,u,w]</td>
<td>x,x+1/2,z [u,u,w]</td>
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</table>

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Symmetry of Special Projections

Along [0,0,1] p4'm'm
\[ \mathbf{a}^* = \frac{(\mathbf{a} - \mathbf{b})}{2}, \quad \mathbf{b}^* = \frac{(\mathbf{a} + \mathbf{b})}{2} \]
Origin at 0,0,z

Along [1,0,0] p2m'2m'g'
\[ \mathbf{a}^* = \mathbf{b}, \quad \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x,1/4,1/4

Along [1,1,0] p2m'm'
\[ \mathbf{a}^* = \frac{-(\mathbf{a} + \mathbf{b})}{2}, \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,x,1/4
Origin at \( \overline{4}c'g' \), at -1/4,1/4,-1/4 from center (2/m')

Asymmetric unit  
\[ 0 \leq x \leq 1/4; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x < y; \quad y < 1/2 - x \]

Symmetry Operations

1. 1
   (1) 1
   (1 0 0)

2. 2 0 0, z
   (2) 2 0 0, z
   (2z 0 0, 0)

3. \( 4' \) (0, 0, 1/2) 0, 1/2, z
   (3) \( 4' \) (0, 0, 1/2) 0, 1/2, z
   (4z 1/2, 1/2, 1/2)

4. \( 4' \) (0, 0, 1/2) 1/2, 0, z
   (4' \( 1/2, 1/2, 1/2 \))

5. (0, 1/2, 0) 1/4, y, 0
   (5) (0, 1/2, 0) 1/4, y, 0
   (2y 1/2, 1/2, 0)

6. \( 4' \) (0, 1/2, 0) x, 1/4, 0
   (6) (0, 1/2, 0) x, 1/4, 0
   (2x 1/2, 1/2, 0)

7. \( 4' \) (0, 0, 1/2) 0, 0, z
   (7) \( 4' \) (0, 0, 1/2) 0, 0, z
   (4z 0, 0, 1/2)

8. \( 4' \) (0, 0, 1/2) 0, 0, z
   (8) \( 4' \) (0, 0, 1/2) 0, 0, z
   (2z 0, 0, 1/2)

9. (1/4, 1/4, 1/4)
   (9) (1/4, 1/4, 1/4)
   (4z 0, 0, 0)

10. (1/2, 1/2, 0)
    (10) (1/2, 1/2, 0) x, y, 1/4
        (mz 1/2, 1/2, 1/2)

11. (1/2, 1/2, 0)
    (11) (1/2, 1/2, 0) x, y, 1/4
        (mz 1/2, 1/2, 1/2)

12. (1/2, 1/2, 0)
    (12) (1/2, 1/2, 0) x, y, 1/4
        (mz 1/2, 1/2, 1/2)

13. (0, 0, 1/2)
    (13) (0, 0, 1/2) x, 0, z
        (my 0, 0, 1/2)

14. (0, 0, 1/2)
    (14) (0, 0, 1/2) 0, y, z
        (mz 0, 0, 1/2)

15. (0, 0, 1/2)
    (15) (0, 0, 1/2) x, 1/2, x, z
        (mz 0, 0, 1/2)

16. (0, 0, 1/2)
    (16) (0, 0, 1/2) x, x, z
        (my 1/2, 1/2, 0)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (9).

<table>
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<td>16</td>
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</tr>
<tr>
<td>(5) x+1/2,y+1/2,z [u,v,w]</td>
<td>(6) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(9) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(10) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(11) y,x,z [v,u,w]</td>
<td>(12) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(13) x,y,z+1/2 [u,v,w]</td>
<td>(14) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(15) y+1/2,x+1/2,z [v,u,w]</td>
<td>(16) y+1/2,x+1/2,z [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>i</td>
</tr>
<tr>
<td>x,x+1/2,z [u,u,w]</td>
<td>x,x+1/2,z [u,u,w]</td>
</tr>
<tr>
<td>x+1/2,x,z [u,u,w]</td>
<td>x+1/2,x,z [u,u,w]</td>
</tr>
<tr>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>8</td>
<td>h</td>
</tr>
<tr>
<td>x,x,3/4 [u,u,0]</td>
<td>x,x,3/4 [u,u,0]</td>
</tr>
<tr>
<td>x+1/2,x,1/4 [u,u,0]</td>
<td>x+1/2,x,1/4 [u,u,0]</td>
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<tr>
<td>x+1/2,1/4 [u,u,0]</td>
<td>x+1/2,1/4 [u,u,0]</td>
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<td>8</td>
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<td>x,x,1/4 [u,u,0]</td>
<td>x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td>x+1/2,x,3/4 [u,u,0]</td>
<td>x+1/2,x,3/4 [u,u,0]</td>
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<td>x+1/2,1/4 [u,u,0]</td>
<td>x+1/2,1/4 [u,u,0]</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
</tr>
<tr>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
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<tr>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
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<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>2,0,z+1/2 [0,0,w]</td>
<td>2,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
</tr>
<tr>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>3/4,1/4,3/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
</tr>
<tr>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
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<tr>
<td>3/4,1/4,3/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
</tr>
<tr>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
</tr>
<tr>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>1/2,1/2,3/4 [0,0,0]</td>
<td>1/2,1/2,3/4 [0,0,0]</td>
</tr>
<tr>
<td>0,0,3/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p4m'm'
\[ a^* = \frac{(a - b)}{2}, \quad b^* = \frac{(a + b)}{2} \]
Origin at 0,0,z

Along [1,0,0] p2m'g'
\[ a^* = b, \quad b^* = \frac{c}{2} \]
Origin at x,1/4,0

Along [1,1,0] p2m'm'
\[ a^* = \frac{(-a + b)}{2}, \quad b^* = c \]
Origin at x,x,1/4
Origin at center (4/mmm)

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x < y\]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\)
   \((1|0,0,0)\)

2. \(2\)
   \((0,0,z)\)
   \((2_z|0,0,0)\)

3. \(4^+\)
   \((0,0,z)\)
   \((4_z|0,0,0)\)

4. \(4^-\)
   \((0,0,z)\)
   \((4_z^{-1}|0,0,0)\)

5. \(2\)
   \((0,y,0)\)
   \((2_y|0,0,0)\)

6. \(2\)
   \((x,0,0)\)
   \((2_x|0,0,0)\)

7. \(2\)
   \((x,x,0)\)
   \((2_{xy}|0,0,0)\)

8. \(m\)
   \((x,y,0)\)
   \((m_x|0,0,0)\)

9. \(m\)
   \((0,y,0)\)
   \((m_y|0,0,0)\)

10. \(m\)
    \((x,0,z)\)
    \((m_x|0,0,0)\)

11. \(m\)
    \((x,x,0)\)
    \((m_{xy}|0,0,0)\)

12. \(m\)
    \((0,0,z)\)
    \((m_{z}|0,0,0)\)
Continued

For $(1/2,1/2,1/2) + \text{ set}$

(1) $t (1/2,1/2,1/2)$  
(1) $2 (0,0,1/2)$  
(1) $4^* (0,0,1/2)$  
(1) $4^* (0,0,1/2)$  
(1) $1/2,0,z$

(2) $2 (1/2,1/2,1/2)$  
(2) $2 (1/2,1/2,1/2)$  
(2) $2 (1/2,1/2,1/2)$  
(2) $2 (1/2,1/2,1/2)$  
(2) $1/2,0,z$

(3) $4^* (0,0,1/2)$  
(3) $4^* (0,0,1/2)$  
(3) $4^* (0,0,1/2)$  
(3) $4^* (0,0,1/2)$  
(3) $1/2,0,z$

(4) $4^* (0,0,1/2)$  
(4) $4^* (0,0,1/2)$  
(4) $4^* (0,0,1/2)$  
(4) $4^* (0,0,1/2)$  
(4) $1/2,0,z$

Generators selected  
(1); $t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>o 1</td>
<td>$(1) x,y,z [u,v,w]$</td>
<td>$(0,0,0) + (1/2,1/2,1/2) +$</td>
</tr>
<tr>
<td>16</td>
<td>n.m.</td>
<td>$(5) x,y,z [u,v,w]$</td>
<td>$(0,0,0)$</td>
</tr>
<tr>
<td>16</td>
<td>m ..m</td>
<td>$(9) x,y,z [u,v,w]$</td>
<td>$0,y,z [u,0,0]$</td>
</tr>
<tr>
<td>16</td>
<td>l ..m</td>
<td>$(10) x,y,z [u,v,w]$</td>
<td>$x,x,z [u,u,0]$</td>
</tr>
<tr>
<td>16</td>
<td>k ..2</td>
<td>$(11) x,y,z [u,v,w]$</td>
<td>$y,x,z [v,u,w]$</td>
</tr>
<tr>
<td>8</td>
<td>j m2m.</td>
<td>$(12) y,z [v,u,w]$</td>
<td>$y,x,z [v,u,w]$</td>
</tr>
<tr>
<td>8</td>
<td>i m2m.</td>
<td>$(13) x,y,z [u,v,w]$</td>
<td>$y,x,z [v,u,w]$</td>
</tr>
<tr>
<td>8</td>
<td>h m2m.</td>
<td>$(14) x,y,z [u,v,w]$</td>
<td>$y,x,z [v,u,w]$</td>
</tr>
<tr>
<td>8</td>
<td>g 2mm.</td>
<td>$(15) x,y,z [u,v,w]$</td>
<td>$y,x,z [v,u,w]$</td>
</tr>
<tr>
<td>8</td>
<td>f ..2/m</td>
<td>$(16) y,x,z [v,u,w]$</td>
<td>$y,x,z [v,u,w]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>-----</td>
<td>---</td>
<td>--------------</td>
<td>---------------</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>4mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>4/mmm 1'</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>mm. 1'</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4/mmm 1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4/mmm 1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1'</th>
<th>Along [1,0,0] c2mm1'</th>
<th>Along [1,1,0] p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{a}^* = \frac{\mathbf{a} - \mathbf{b}}{2} ) \quad \mathbf{b}^* = \frac{\mathbf{a} + \mathbf{b}}{2}</td>
<td>\mathbf{a}^* = \mathbf{b} \quad \mathbf{b}^* = \mathbf{c}</td>
<td>\mathbf{a}^* = -\frac{\mathbf{a} + \mathbf{b}}{2} \quad \mathbf{b}^* = \frac{\mathbf{c}}{2}</td>
</tr>
<tr>
<td>Origin at 0,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin at center \((4/mmm1')\)

Asymmetric unit \(0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/4; \ x \leq y\)

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix} \\
(2) & \begin{pmatrix} 2 \\ 0,0,z \\ 2z,0,0,0 \end{pmatrix} \\
(3) & \begin{pmatrix} 4^+ \\ 0,0,z \\ 4z,0,0,0 \end{pmatrix} \\
(4) & \begin{pmatrix} 4^- \\ 0,0,z \\ 4z^{-1},0,0,0 \end{pmatrix} \\
(5) & \begin{pmatrix} 2 \\ 0,y,0 \\ 2y,0,0,0 \end{pmatrix} \\
(6) & \begin{pmatrix} 2 \\ x,0,0 \\ 2x,0,0,0 \end{pmatrix} \\
(7) & \begin{pmatrix} 2 \\ x,x,0 \\ 2zx,0,0,0 \end{pmatrix} \\
(8) & \begin{pmatrix} 2 \\ x,x,0 \\ 2x,0,0,0 \end{pmatrix} \\
(9) & \begin{pmatrix} \bar{1} \\ 0,0,0 \end{pmatrix} \\
(10) & \begin{pmatrix} m \\ x,y,0 \\ m_y,0,0,0 \end{pmatrix} \\
(11) & \begin{pmatrix} \bar{4}^+ \\ 0,0,z \\ \bar{4}z,0,0,0 \end{pmatrix} \\
(12) & \begin{pmatrix} \bar{4}^- \\ 0,0,z \\ \bar{4}z^{-1},0,0,0 \end{pmatrix} \\
(13) & \begin{pmatrix} m \\ x,0,z \\ m_y,0,0,0 \end{pmatrix} \\
(14) & \begin{pmatrix} m \\ 0,y,z \\ m_y,0,0,0 \end{pmatrix} \\
(15) & \begin{pmatrix} m \\ x,x,z \\ m_{xy},0,0,0 \end{pmatrix} \\
(16) & \begin{pmatrix} m \\ x,x,z \\ m_{xy},0,0,0 \end{pmatrix}
\end{align*}
\]
Continued

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (2) 2 (0,0,1/2) 1/4,1/4,z (3) 4^+ (0,0,1/2) 0,1/2,z (4) 4^- (0,0,1/2) 1/2,0,z
   (1/2,1/2,1/2) (2z 1/2,1/2,1/2) (4z 1/2,1/2,1/2) (4z^-1 1/2,1/2,1/2)

(5) 2 (0,1/2,0) 1/4,y,1/4 (6) 2 (1/2,0,0) x,1/4,1/4 (7) 2 (1/2,1/2,0) x,x,1/4
   (2z 1/2,1/2,1/2) (2z 1/2,1/2,1/2) (2x 1/2,1/2,1/2)

(9) T 1/4,1/4,1/4 (10) n (1/2,1/2,0) x,y,1/4 (11) 4^- 1/2,0,z; 1/2,0,1/4
   (T 1/2,1/2,1/2) (mz 1/2,1/2,1/2) (4z^-1 1/2,1/2,1/2)

(13) n (1/2,0,1/2) x,1/4,z (mz 1/2,1/2,1/2) (14) n (0,1/2,1/2) 1/4,y,z (15) c (0,0,1/2) x+1/2,x

   (mz 1/2,1/2,1/2) (mx 1/2,1/2,1/2) (mxy 1/2,1/2,1/2)

For (0,0,0)' + set

(1') 1' (2') 0,0,z (3') 4'^+ 0,0,z (4') 4'^- 0,0,z
   (1' 0,0,0)' (2' 0,0,0)' (4' 0,0,0)' (4' 0,0,0)' (4' 0,0,0)' (4' 0,0,0)' (4' 0,0,0)'

(5') 2' 0,y,0 (6') 2' x,0,0 (7') 2' x,x,0
   (2'y 0,0,0)' (2'z 0,0,0)' (2'z 0,0,0)'

(9') T' 0,0,0 (10') m' x,y,0 (11') 4'^- 0,0,z; 0,0,0
   (T' 0,0,0)' (m'z 0,0,0)' (4'z^-1 0,0,0)'

(13') m' x,0,z (mz 0,0,0)' (14') m' 0,y,z (m'z 0,0,0)' (15') m' x,x,z (m'xy 0,0,0)'

   (mz 1/2,1/2,1/2) (mx 0,0,0)' (m'x 0,0,0)'

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (2) 2' (0,0,1/2) 1/4,1/4,z (3) 4'^+ (0,0,1/2) 0,1/2,z (4) 4'^- (0,0,1/2) 1/2,0,z
   (1/2,1/2,1/2)' (2z 1/2,1/2,1/2)' (4z 1/2,1/2,1/2)' (4z^-1 1/2,1/2,1/2)'

(5') 2' (0,1/2,0) 1/4,y,1/4 (6') 2' (1/2,0,0) x,1/4,1/4 (7') 2' (1/2,1/2,0) x,x,1/4
   (2z 1/2,1/2,1/2)' (2z 1/2,1/2,1/2)' (2x 1/2,1/2,1/2)'

(9') T' 1/4,1/4,1/4 (10') n' (1/2,1/2,0) x,y,1/4 (11') 4'^- 1/2,0,z; 1/2,0,1/4
   (T' 1/2,1/2,1/2)' (mz 1/2,1/2,1/2)' (4z^-1 1/2,1/2,1/2)'

(13') n' (1/2,0,1/2) x,1/4,z (mz 1/2,1/2,1/2)' (14') n' (0,1/2,1/2) 1/4,y,z (15') c' (0,0,1/2) x+1/2,x

   (mz 1/2,1/2,1/2)' (mx 1/2,1/2,1/2)' (m'xy 1/2,1/2,1/2)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

(0,0,0)' + (1/2,1/2,1/2)' +
32  o  11' (1) x,y,z [0,0,0]  (2) \bar{x},\bar{y},z [0,0,0]  (3) y,x,z [0,0,0]  (4) y,\bar{x},z [0,0,0]  \\
(5) x,\bar{y},z [0,0,0]  (6) x,\bar{y},z [0,0,0]  (7) y,\bar{x},z [0,0,0]  (8) y,\bar{x},z [0,0,0]  \\
(9) x,\bar{y},z [0,0,0]  (10) x,\bar{y},z [0,0,0]  (11) y,\bar{x},z [0,0,0]  (12) y,\bar{x},z [0,0,0]  \\
(13) x,\bar{y},z [0,0,0]  (14) x,\bar{y},z [0,0,0]  (15) y,\bar{x},z [0,0,0]  (16) y,\bar{x},z [0,0,0]  \\
16  n  .m.1' 0,y,z [0,0,0]  (0,y,z [0,0,0]  (y,0,z [0,0,0])  \\
(0,y,z [0,0,0]  (0,y,z [0,0,0]  (y,0,z [0,0,0]  (y,0,z [0,0,0]  \\
16  m  ..m1' x,x,z [0,0,0]  (x,x,z [0,0,0]  (x,x,z [0,0,0]  \\
(x,x,z [0,0,0]  (x,x,z [0,0,0]  (x,x,z [0,0,0]  (x,x,z [0,0,0]  \\
16  l  m..1' x,y,0 [0,0,0]  (x,y,0 [0,0,0]  (y,x,0 [0,0,0]  \\
(x,y,0 [0,0,0]  (x,y,0 [0,0,0]  (y,x,0 [0,0,0]  (y,x,0 [0,0,0]  \\
16  k  ..21' x,x+1/2,1/4 [0,0,0]  (x,x+1/2,1/4 [0,0,0]  (x,x+1/2,1/4 [0,0,0]  \\
(x,x+1/2,1/4 [0,0,0]  (x,x+1/2,1/4 [0,0,0]  (x,x+1/2,1/4 [0,0,0]  (x,x+1/2,1/4 [0,0,0]  \\
8  j  m2m.1' x,1/2,0 [0,0,0]  (x,1/2,0 [0,0,0]  (1/2,x,0 [0,0,0]  \\
(x,1/2,0 [0,0,0]  (x,1/2,0 [0,0,0]  (1/2,x,0 [0,0,0]  (1/2,x,0 [0,0,0]  \\
8  i  m2m.1' x,0,0 [0,0,0]  (x,0,0 [0,0,0]  (0,x,0 [0,0,0]  \\
(x,0,0 [0,0,0]  (x,0,0 [0,0,0]  (0,x,0 [0,0,0]  (0,x,0 [0,0,0]  \\
8  h  m.2m1' x,x,0 [0,0,0]  (x,x,0 [0,0,0]  (x,x,0 [0,0,0]  \\
(x,x,0 [0,0,0]  (x,x,0 [0,0,0]  (x,x,0 [0,0,0]  (x,x,0 [0,0,0]  \\
8  g  2mm.1' 0,1/2,z [0,0,0]  (1/2,0,z [0,0,0]  (0,1/2,z [0,0,0]  \\
(0,1/2,z [0,0,0]  (0,1/2,z [0,0,0]  (0,1/2,z [0,0,0]  (0,1/2,z [0,0,0]  \\
8  f  ..2/m1' 1/4,1/4,1/4 [0,0,0]  (3/4,3/4,1/4 [0,0,0]  (3/4,1/4,1/4 [0,0,0]  \\
(3/4,1/4,1/4 [0,0,0]  (3/4,1/4,1/4 [0,0,0]  (3/4,1/4,1/4 [0,0,0]  (3/4,1/4,1/4 [0,0,0]  \\
4  e  4mm1' 0,0,z [0,0,0]  (0,0,z [0,0,0]  \\
4  d  4mm1' 0,1/2,1/4 [0,0,0]  (1/2,0,1/4 [0,0,0]  \\
4  c  4mm1' 0,1/2,0 [0,0,0]  (1/2,0,0 [0,0,0]  \\
2  b  4mm1' 0,0,0 [0,0,0]  \\
2  a  4mm1' 0,0,0 [0,0,0]  \\

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1'</th>
<th>Along [1,0,0] c2mm1'</th>
<th>Along [1,1,0] p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>a* = b</td>
<td>a* = (-a + b)/2</td>
</tr>
<tr>
<td>b* = (a + b)/2</td>
<td>b* = c</td>
<td>b* = c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
Origin at x,0,0
Origin at x,x,0
Origin at center (4/m'mm)

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x < y

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(5) 2' 0,y,0
(2y|0,0,0)'

(9) T' 0,0,0
(1|0,0,0)'

(13) m x,0,z
(m|0,0,0)

(2) 2 0,0,z
(2z|0,0,0)

(6) 2' x,0,0
(2x|0,0,0)'

(10) m' x,y,0
(mz|0,0,0)'

(3) 4' 0,0,z
(4z|0,0,0)

(7) 2' x,x,0
(2xy|0,0,0)'

(11) 4'' 0,0,z; 0,0,0
(4z|0,0,0)'

(14) m 0,y,z
(mz|0,0,0)

(4) 4' 0,0,z
(4z|0,0,0)

(8) 2' x,x,0
(2xy|0,0,0)'

(12) 4'' 0,0,z; 0,0,0
(4z|0,0,0)'

(15) m x,x,z
(mxy|0,0,0)

(16) m x,x,z
(mxy|0,0,0)
Continued

<table>
<thead>
<tr>
<th>(1) t (1/2,1/2,1/2)</th>
<th>(2) t (1/2,1/2,1/2)</th>
<th>(3) t (1/2,1/2,1/2)</th>
<th>(4) t (1/2,1/2,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (1/2,1/2,1/2)</td>
<td>(2) t (1/2,1/2,1/2)</td>
<td>(3) t (1/2,1/2,1/2)</td>
<td>(4) t (1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(5) 2' (0,1/2,0) 1/4,y,1/4</td>
<td>(6) 2' (0,1/2,0) 1/4,y,1/4</td>
<td>(7) 2' (0,1/2,0) 1/4,y,1/4</td>
<td>(8) 2' (0,1/2,0) 1/4,y,1/4</td>
</tr>
<tr>
<td>(5) 2' (0,1/2,0) 1/4,y,1/4</td>
<td>(6) 2' (0,1/2,0) 1/4,y,1/4</td>
<td>(7) 2' (0,1/2,0) 1/4,y,1/4</td>
<td>(8) 2' (0,1/2,0) 1/4,y,1/4</td>
</tr>
<tr>
<td>(9) T 1/2,1/2,1/2'</td>
<td>(10) n' (1/2,1/2,1/2) x,y,z</td>
<td>(11) 4^+ 1/2,0,z 1/2,0,1/4</td>
<td>(12) 4^- 1/2,1/2,1/2'</td>
</tr>
<tr>
<td>(9) T 1/2,1/2,1/2'</td>
<td>(10) n' (1/2,1/2,1/2) x,y,z</td>
<td>(11) 4^+ 1/2,0,z 1/2,0,1/4</td>
<td>(12) 4^- 1/2,1/2,1/2'</td>
</tr>
<tr>
<td>(13) n (1/2,0,1/2) x,1/4,z</td>
<td>(14) n (0,1/2,1/2) 1/4,y,z</td>
<td>(15) c (0,0,1/2) x+1/2,x,z</td>
<td>(16) n (1/2,1/2,1/2) x,x,z</td>
</tr>
<tr>
<td>(13) n (1/2,0,1/2) x,1/4,z</td>
<td>(14) n (0,1/2,1/2) 1/4,y,z</td>
<td>(15) c (0,0,1/2) x+1/2,x,z</td>
<td>(16) n (1/2,1/2,1/2) x,x,z</td>
</tr>
</tbody>
</table>

Generators selected

| (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9). |

Positions

| Multiplicity, Wyckoff letter, Site Symmetry. |

| Coordinates |

| (0,0,0) + | (1/2,1/2,1/2) + |

<table>
<thead>
<tr>
<th>32 o 1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) x,y,z [u,v,w]</th>
<th>(3) x,y,z [v,u,w]</th>
<th>(4) x,y,z [v,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 n .m. 0,y,z [u,0,0]</td>
<td>0,y,z [u,0,0]</td>
<td>y,0,z [0,u,0]</td>
<td>y,0,z [0,u,0]</td>
<td></td>
</tr>
<tr>
<td>16 m ..m x,x,z [u,0,0]</td>
<td>x,x,z [u,0,0]</td>
<td>x,x,z [u,0,0]</td>
<td>x,x,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td>16 l m'.. x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
<td>y,x,0 [v,u,0]</td>
<td>y,x,0 [v,u,0]</td>
<td></td>
</tr>
<tr>
<td>16 k ..2' x,x+1/2,1/4 [u,u,w]</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
<td>x+1/2,x,1/4 [u,u,w]</td>
<td>x+1/2,x,1/4 [u,u,w]</td>
<td></td>
</tr>
<tr>
<td>8 j m'2.m. x,1/2,0 [0,v,0]</td>
<td>x,1/2,0 [0,v,0]</td>
<td>1/2,x,0 [v,0,0]</td>
<td>1/2,x,0 [v,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 i m'2.m. x,0,0 [0,v,0]</td>
<td>x,0,0 [0,v,0]</td>
<td>x,0,0 [0,v,0]</td>
<td>x,0,0 [0,v,0]</td>
<td></td>
</tr>
<tr>
<td>8 h m'2'm x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>8 g 2mm. 0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 f ..2'm 1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>
4    e    4mm    0,0,z [0,0,0]    0,0,z [0,0,0]

4    d    4\_m2'    0,1/2,1/4 [0,0,0]    1/2,0,1/4 [0,0,0]

4    c    m'\_mm.    0,1/2,0 [0,0,0]    1/2,0,0 [0,0,0]

2    b    4/m'\_mm    0,0,1/2 [0,0,0]

2    a    4/m'\_mm    0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] c2mm1'
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along [1,1,0] p2mm1'
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
I4'/mm'm
139.4.1182

4'/mm'm

Tetragonal
I4'/m2'/m'2/m

Origin at center (4'/mm'm)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ y

Symmetry Operations
For (0,0,0) + set

(1) 1
(1 0,0,0)

(5) 2' 0,y,0
(2z 0,0,0)'

(9) 1 0,0,0
(1 0,0,0)

(13) m' x,0,z
(m 0,0,0)'

(2) 2 0,0,z
(2z 0,0,0)

(6) 2' x,0,0
(2z 0,0,0)'

(10) m x,y,0
(m 0,0,0)

(14) m' 0,y,z
(m 0,0,0)'

(3) 4' 0,0,z
(4z 0,0,0)'

(7) 2 x,x,0
(2xy 0,0,0)

(11) 4' 0,0,z
(4z 0,0,0)'

(8) 2 x,x,0
(2xy 0,0,0)

(12) 4' 0,0,z
(4z 0,0,0)'

(15) m x,x,0
(mxy 0,0,0)

(16) m x,x,0
(mxy 0,0,0)
Continued

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  (2) 2 (0,0,1/2)  (3) 4* (0,0,1/2)  (4) 4* (0,0,1/2) 
(1/2,1/2,1/2)  1/4,1/4,z  0,1/2,z  1/2,0,z

(5) 2' (0,1/2,0)  1/4,y,1/4  (6) 2' (1/2,0,0)  x,1/4,1/4  (7) 2 (1/2,1/2,0)  x,x,1/4  (8) 2 x, x+1/2,1/4 
(2',1/2,1/2,1/2)  (2',1/2,1/2,1/2)  1/2,1/2,1/2)  1/2,1/2,1/2)

(9) 1/4,1/4,1/4  (10) n (1/2,1/2,0)  x,y,z  (11) 4* ' 1/2,0,1/4  (12) 4* ' 0,1/2,1/2  (13) n' (1/2,0,1/2)  x,1/4,z  (14) n' (0,1/2,1/2)  1/4,y,z  (15) c (0,0,1/2)  x+1/2,x  (16) n (1/2,1/2,1/2)  x,1/2,1/2,1/2)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter, Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>16 n .m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>y,0,z [v,0,w]</td>
</tr>
<tr>
<td></td>
<td>y,0,z [v,0,w]</td>
</tr>
<tr>
<td>16 m .m</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
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<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
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<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>16 l .m</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>y,x,0 [0,0,w]</td>
</tr>
<tr>
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<td>y,x,0 [0,0,w]</td>
</tr>
<tr>
<td>16 k .2</td>
<td>x,x+1/2,1/4 [u,u,0]</td>
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<tr>
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<td>x,x+1/2,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x+1/2,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td>8 j m2m'</td>
<td>x,1/2,0 [0,0,w]</td>
</tr>
<tr>
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<td>x,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,x,0 [0,0,w]</td>
</tr>
<tr>
<td>8 i m2m'</td>
<td>x,0,0 [0,0,w]</td>
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<tr>
<td></td>
<td>x,0,0 [0,0,w]</td>
</tr>
<tr>
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<td>0,x,0 [0,0,w]</td>
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<td>0,x,0 [0,0,w]</td>
</tr>
<tr>
<td>8 h m.2m</td>
<td>x,x,0 [0,0,0]</td>
</tr>
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<td>x,x,0 [0,0,0]</td>
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<td>x,x,0 [0,0,0]</td>
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<td>x,x,0 [0,0,0]</td>
</tr>
<tr>
<td>8 g 2m'</td>
<td>0,1/2,z [0,0,w]</td>
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<td>0,1/2,z [0,0,w]</td>
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<td>1/2,0,z [0,0,w]</td>
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<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 f ..2/m</td>
<td>1/4,1/4,1/4 [u,u,0]</td>
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<td>3/4,3/4,1/4 [u,u,0]</td>
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<td>3/4,3/4,1/4 [u,u,0]</td>
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<td>1/4,3/4,1/4 [u,u,0]</td>
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</tbody>
</table>

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Symmetry of Special Projections

<table>
<thead>
<tr>
<th>沿 [0,0,1] p4mm1'</th>
<th>沿 [1,0,0] c2'mm'</th>
<th>沿 [1,1,0] p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>a = (a - b)/2  b</em> = (a + b)/2</td>
<td><em>a = b  b</em> = c</td>
<td><em>a = (-a + b)/2  b</em> = c/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin at center (4/mmm')

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≥ y

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2|0,0,0)

(3) 4' 0,0,z
(4|0,0,0)

(4) 4' 0,0,z
(4|0,0,0)

(5) 2 0,y,0
(2|0,0,0)

(6) 2 x,0,0
(2|0,0,0)

(7) 2' x,x,0
(2|0,0,0)

(8) 2' x,x,0
(2|0,0,0)

(9) m 0,0,0
(1|0,0,0)

(10) m x,y,0
(m|0,0,0)

(11) 4* 0,0,z
(4|0,0,0)

(12) 4* 0,0,z
(4|0,0,0)

(13) m x,0,z
(m|0,0,0)

(14) m 0,y,z
(m|0,0,0)

(15) m' x,x,z
(m|0,0,0)

(16) m' x,x,z
(m|0,0,0)
For $(1/2,1/2,1/2) + \text{set}$

(1) $t\ (1/2,1/2,1/2)
(1/2,1/2,1/2)$

(2) $2\ (0,0,1/2)\ 1/4,1/4,z$

(3) $4^+\ (0,0,1/2)\ 0,1/2,z$

(4) $4^-\ (0,0,1/2)\ 1/2,0,z$

(5) $2\ (0,1/2,0)\ 1/4,y,1/4$

(6) $2\ (1/2,0,0)\ x,1/4,1/4$

(7) $2'\ (1/2,1/2,0)\ x,x,1/4$

(8) $2^-\ x,x+1/2,1/4$

(9) $\overline{1}\ 1/4,1/4,1/4$

(10) $n\ (1/2,1/2,0)\ x,y,1/4$

(11) $4^-\ 1/2,0,z; 1/2,0,1/4$

(12) $\overline{4}^-\ 0,1/2,z; 0,1/2,1/4$

(13) $n\ (1/2,0,1/2)\ x,1/4,z$

(14) $n\ (0,1/2,1/2)\ 1/4,y,z$

(15) $c\ (0,0,1/2)\ x+1/2,x,z$

(16) $n'\ (1/2,1/2,1/2)\ x,x,z$

Generators selected

(1); $t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(1/2,1/2,1/2) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>y,x,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(9) x,y,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(13) x,y,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(16) y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
</tbody>
</table>

18 m .m'

16 l ..m.

16 k ..2'

8 j m2m.

8 i m2m.

8 h m.2'm'

8 g 2mm.

8 f ..2'/m'

Continued
Symmetry of Special Projections

Along [0,0,1] p4mm1'  
\( a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \)  
Origin at 0,0,z

Along [1,0,0] c2mm1'  
\( a^* = b \quad b^* = c \)  
Origin at x,0,0

Along [1,1,0] p2'mm'  
\( a^* = -\frac{c}{2} \quad b^* = \frac{(-a + b)}{2} \)  
Origin at x,x,0
Origin at center (4'/m'm'm)

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ y

Symmetry Operations

For (0,0,0) + set

1. 1
   (1) 0,0,0

2. 2' 0,0,z
   (2) x,0,0
   (2x,0,0)

3. 4' 0,0,z
   (3) z,0,0
   (4z,0,0)

4. 4' 0,0,z
   (4) z,0,0
   (4z,0,0)

5. 2 0,y,0
   (2y,0,0)

6. 2' 0,z,0
   (2z,0,0)

7. 2' x,x,0
   (2x,0,0)

8. 2' x,x,0
   (2x,0,0)

9. 1 0,0,0
   (1) 0,0,0

10. m' x,y,0
    (10) x,y,0
    (mz,0,0)

11. 4' z,0,0
    (11) 0,0,z
    (4z,0,0)

12. 4' z,0,0
    (12) 0,0,z
    (4z,0,0)

13. m' x,0,z
    (mz,0,0)

14. m' 0,0,z
    (14) x,0,0
    (mz,0,0)

15. m x,x,0
    (15) x,y,0
    (mz,0,0)

16. m x,x,0
    (16) x,y,0
    (mz,0,0)
For \((1/2,1/2,1/2) + \) set

<table>
<thead>
<tr>
<th>((1/2,1/2,1/2) + )</th>
<th>((1/2,1/2,1/2) + )</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1)) t ((1/2,1/2,1/2))</td>
<td>((1)) t ((1,0,0))</td>
</tr>
<tr>
<td>((2)) 2 ((0,0,1/2))</td>
<td>((2)) t ((0,1,0))</td>
</tr>
<tr>
<td>((3)) 4(\cdot) ((0,0,1/2)) ((0,1/2,z))</td>
<td>((3)) 4(\cdot) ((0,0,1/2)) ((1/2,0,z))</td>
</tr>
<tr>
<td>((4)) 4(\cdot) ((0,0,1/2)) ((1/2,1/2,1/2))</td>
<td>((4)) 4(\cdot) ((0,0,1/2)) ((1/2,1/2,1/2))</td>
</tr>
</tbody>
</table>

Generators selected  
\((1)\); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(1/2,1/2,1/2)\); \((2)\); \((3)\); \((5)\); \((9)\).

**Positions**

**Multiplicity,**  
Wyckoff letter,  
Site Symmetry letter.

<table>
<thead>
<tr>
<th>((0,0,0) + )</th>
<th>((1/2,1/2,1/2) + )</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 o 1 ((1)) x, y, z ([u,v,w])</td>
<td>((3)) y, x, z ([v,u,w])</td>
</tr>
<tr>
<td>((5)) x, y, z ([u,v,w])</td>
<td>((7)) y, x, z ([v,u,w])</td>
</tr>
<tr>
<td>((6)) x, y, z ([u,v,w])</td>
<td>((8)) y, x, z ([v,u,w])</td>
</tr>
<tr>
<td>((9)) x, y, z ([u,v,w])</td>
<td>((10)) x, y, z ([u,v,w])</td>
</tr>
<tr>
<td>((11)) y, x, z ([v,u,w])</td>
<td>((12)) y, x, z ([v,u,w])</td>
</tr>
<tr>
<td>((13)) x, y, z ([u,v,w])</td>
<td>((14)) x, y, z ([u,v,w])</td>
</tr>
<tr>
<td>((15)) y, x, z ([v,u,w])</td>
<td>((16)) y, x, z ([v,u,w])</td>
</tr>
</tbody>
</table>

| 16 n \(\cdot m'\) | \(0, y, z [0, v, w]\) |
| \(0, y, z [0, v, w]\) | \(y, 0, z [v, 0, w]\) |
| \(y, 0, z [v, 0, w]\) | \(y, 0, z [v, 0, w]\) |

| 16 m \(\cdot m\) | \([x, x, z [u, u, 0]\) |
| \([x, x, z [u, u, 0]\) | \([x, x, z [u, u, 0]\) |
| \([x, x, z [u, u, 0]\) | \([x, x, z [u, u, 0]\) |

| 16 l \(\cdot m'\) | \(x, y, z [u,v,0]\) |
| \(x, y, z [u,v,0]\) | \(y, x, z [v,u,0]\) |
| \(y, x, z [v,u,0]\) | \(y, x, z [v,u,0]\) |

| 16 k \(\cdot 2'\) | \(x,x+1/2,1/4 [u,u,w]\) |
| \(x,x+1/2,1/4 [u,u,w]\) | \(x+1/2,x,1/4 [u,u,w]\) |
| \(x+1/2,x,1/4 [u,u,w]\) | \(x+1/2,x,3/4 [u,u,w]\) |

| 8 j \(m'2m'\) | \(x,1/2,0 [u,0,0]\) |
| \(x,1/2,0 [u,0,0]\) | \(1/2,x,0 [0,1,u,0]\) |
| \(1/2,x,0 [0,1,u,0]\) | \(1/2,x,0 [0,1,u,0]\) |

| 8 i \(m'2m'\) | \(x,0,0 [u,0,0]\) |
| \(x,0,0 [u,0,0]\) | \(0,x,0 [0,u,0]\) |
| \(0,x,0 [0,u,0]\) | \(0,x,0 [0,u,0]\) |

| 8 h \(m'2m'\) | \(x,0,0 [u,0,0]\) |
| \(x,0,0 [u,0,0]\) | \(x,x,0 [u,0,0]\) |
| \(x,x,0 [u,0,0]\) | \(x,x,0 [u,0,0]\) |

| 8 g \(2m'2m'\) | \(0,1/2,z [0,0,w]\) |
| \(0,1/2,z [0,0,w]\) | \(1/2,0,z [0,0,w]\) |
| \(1/2,0,z [0,0,w]\) | \(1/2,0,z [0,0,w]\) |

| 8 f \(\cdot 2'm\) | \(1/4,1/4,1/4 [0,0,0]\) |
| \(3/4,3/4,1/4 [0,0,0]\) | \(3/4,1/4,1/4 [0,0,0]\) |
| \(3/4,1/4,1/4 [0,0,0]\) | \(1/4,3/4,1/4 [0,0,0]\) |
4  e  4'm'm'  0,0,z [0,0,0]  0,0,z [0,0,0]
4  d  4'm'2'  0,1/2,1/4 [0,0,w]  1/2,0,1/4 [0,0,w]
4  c  m'm'm'  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]
2  b  4'/m'm'm'  0,0,1/2 [0,0,0]
2  a  4'/m'm'm'  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4'mm'
\[a^* = \frac{a - b}{2}\] \[b^* = \frac{a + b}{2}\]
Origin at 0,0,z

Along [1,0,0] c2m'm'
\[a^* = b\] \[b^* = c\]
Origin at x,0,0

Along [1,1,0] p2mm1'
\[a^* = \frac{-a + b}{2}\] \[b^* = \frac{c}{2}\]
Origin at x,x,0
Origin at center (4/mm'm')

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x < y \]

Symmetry Operations

For (0,0,0) + set

1. \( \bar{1} \quad (0,0,0) \)
2. \( \bar{2} \quad 0,0,z \)
3. \( \bar{4} \quad 0,0,z \)
4. \( \bar{4}^{-1} \quad 0,0,z \)
5. \( 2' \quad 0,y,0 \)
6. \( 2' \quad x,0,0 \)
7. \( 2' \quad x,x,0 \)
8. \( 2' \quad x,x,0 \)
9. \( \bar{1} \quad 0,0,0 \)
10. \( \bar{m} \quad x,y,0 \)
11. \( \bar{4} \quad 0,0,z; 0,0,0 \)
12. \( \bar{4}^{-1} \quad 0,0,z; 0,0,0 \)
13. \( \bar{m}' \quad x,0,z \)
14. \( \bar{m}' \quad 0,y,z \)
15. \( \bar{m}' \quad x,x,z \)
16. \( \bar{m}' \quad x,x,z \)
Continued

For \((1/2,1/2,1/2)\) + set

\begin{align*}
(1) & \ t (1/2,1/2,1/2) \\
(2) & \ 2 (0,0,1/2) \\
(3) & \ 4^+ (0,0,1/2) \\
(4) & \ 4^+ (0,0,1/2) \\
& \ t (1/2,1/2,1/2) \\
& \ t (1/2,1/2,1/2) \\
& \ (4^+_z) 1/2,1/2,1/2) \\
(5) & \ 2' (0,1/2,0) \\
(6) & \ 2' (1/2,0,0) \\
(7) & \ 2' (1/2,1/2,0) \\
(8) & \ 2' (0,1/2,1/2) \\
& \ (2,1/2,1/2') \\
& \ (2,1/2,1/2') \\
& \ (2,1/2,1/2') \\
& \ (2,1/2,1/2') \\
& \ (2,1/2,1/2') \\
(9) & \ 1/4,1/4,1/4 \\
(10) & \ 1/4,1/4,1/4 \\
(11) & \ 1/4,1/4,1/4 \\
(12) & \ 1/4,1/4,1/4 \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
(13) & \ 1/4,1/4,1/4 \\
(14) & \ 1/4,1/4,1/4 \\
(15) & \ 1/4,1/4,1/4 \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
(16) & \ 1/4,1/4,1/4 \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
& \ (1/2,1/2,1/2') \\
\end{align*}

Generators selected \((1)\); \((t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9)).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 o 1</td>
<td>((0,0,0) + )</td>
<td>((1/2,1/2,1/2) + )</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z ([u,v,w])</td>
<td>(x, y, z )</td>
<td>([u,v,w])</td>
<td></td>
</tr>
<tr>
<td>(5) (x, y, z )</td>
<td>(0, y, z )</td>
<td>([0, v, w])</td>
<td></td>
</tr>
<tr>
<td>(9) (x, y, z )</td>
<td>(0, y, z )</td>
<td>([0, v, w])</td>
<td></td>
</tr>
<tr>
<td>(13) (x, y, z )</td>
<td>(0, y, z )</td>
<td>([0, v, w])</td>
<td></td>
</tr>
<tr>
<td>16 n .m'</td>
<td>(0, y, z )</td>
<td>([0, v, w])</td>
<td></td>
</tr>
<tr>
<td>(10) (0, y, z )</td>
<td>(y, 0, z )</td>
<td>([0, v, w])</td>
<td></td>
</tr>
<tr>
<td>(14) (0, y, z )</td>
<td>(y, 0, z )</td>
<td>([0, v, w])</td>
<td></td>
</tr>
<tr>
<td>16 m ..m'</td>
<td>(x, x, z )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>(6) (x, x, z )</td>
<td>(x, x, z )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>(10) (x, x, z )</td>
<td>(x, x, z )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>(13) (x, x, z )</td>
<td>(x, x, z )</td>
<td>([u, u, w])</td>
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</tr>
<tr>
<td>16 l m..</td>
<td>(x, x, z )</td>
<td>([0, 0, w])</td>
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<td>(7) (0, x, z )</td>
<td>(0, x, z )</td>
<td>([0, 0, w])</td>
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<tr>
<td>(11) (0, x, z )</td>
<td>(0, x, z )</td>
<td>([0, 0, w])</td>
<td></td>
</tr>
<tr>
<td>(15) (0, x, z )</td>
<td>(0, x, z )</td>
<td>([0, 0, w])</td>
<td></td>
</tr>
<tr>
<td>16 k ..2'</td>
<td>(x, x+1/2,1/4 )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>(8) (x, x+1/2,1/4 )</td>
<td>(x, x+1/2,1/4 )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>(12) (x, x+1/2,1/4 )</td>
<td>(x, x+1/2,1/4 )</td>
<td>([u, u, w])</td>
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</tr>
<tr>
<td>(16) (x, x+1/2,1/4 )</td>
<td>(x, x+1/2,1/4 )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>8 j m2m'</td>
<td>(x, 1/2,0 )</td>
<td>([0, 0, w])</td>
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<tr>
<td>(9) (x, 1/2,0 )</td>
<td>(1/2, x, 0 )</td>
<td>([0, 0, w])</td>
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<td>(13) (x, 1/2,0 )</td>
<td>(1/2, x, 0 )</td>
<td>([0, 0, w])</td>
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<td>8 i m2m'</td>
<td>(x, 0,0 )</td>
<td>([0, 0, w])</td>
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<td>(10) (x, 0,0 )</td>
<td>(0, x, 0 )</td>
<td>([0, 0, w])</td>
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<td>(14) (x, 0,0 )</td>
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<td>([0, 0, w])</td>
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<td>8 h m2m'</td>
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<td>([0, 0, w])</td>
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<tr>
<td>(11) (x, x,0 )</td>
<td>(x, x,0 )</td>
<td>([0, 0, w])</td>
<td></td>
</tr>
<tr>
<td>(15) (x, x,0 )</td>
<td>(x, x,0 )</td>
<td>([0, 0, w])</td>
<td></td>
</tr>
<tr>
<td>8 g 2m'</td>
<td>(0,1/2,z )</td>
<td>([0, 0, w])</td>
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</tr>
<tr>
<td>(12) (0,1/2,z )</td>
<td>(0,1/2,z )</td>
<td>([0, 0, w])</td>
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</tr>
<tr>
<td>(16) (0,1/2,z )</td>
<td>(0,1/2,z )</td>
<td>([0, 0, w])</td>
<td></td>
</tr>
<tr>
<td>8 f ..2/m'</td>
<td>(1/4,1/4,1/4 )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>(13) (1/4,1/4,1/4 )</td>
<td>(3/4,3/4,1/4 )</td>
<td>([u, u, w])</td>
<td></td>
</tr>
<tr>
<td>(14) (1/4,1/4,1/4 )</td>
<td>(3/4,3/4,1/4 )</td>
<td>([u, u, w])</td>
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</table>

139.7.1185 - 2 - 2506
Symmetry of Special Projections

Along [0, 0, 1] p4mm1'  
\[ a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \]
Origin at 0, 0, z

Along [1, 0, 0] c2mm  
\[ a^* = b \quad b^* = c \]
Origin at x, 0, 0

Along [1, 1, 0] p2'mm'  
\[ a^* = -\frac{c}{2} \quad b^* = -\frac{(a + b)}{2} \]
Origin at x, x, 0
I4'/m'2/m'

Origin at center (I4'/m'2/m')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x < y \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \(1 \quad (1|0,0,0)\)
2. \(2 \quad 0,0,z \quad (2_z|0,0,0)\)
3. \(4' \quad 0,0,z \quad (4_z|0,0,0)\)
4. \(4' \quad 0,0,z \quad (4_z^{-1}|0,0,0)\)
5. \(2' \quad 0,y,0 \quad (2_y|0,0,0)\)
6. \(2' \quad x,0,0 \quad (2_x|0,0,0)\)
7. \(2 \quad x,x,0 \quad (2_x|0,0,0)\)
8. \(2 \quad x,x,0 \quad (2_x|0,0,0)\)
9. \(\bar{1}' \quad 0,0,0 \quad (1|0,0,0)\)
10. \(m' \quad x,y,0 \quad (m_z|0,0,0)\)
11. \(\bar{4}^+ \quad 0,0,z; 0,0,0 \quad (\bar{4}_z|0,0,0)\)
12. \(\bar{4}^+ \quad 0,0,z; 0,0,0 \quad (\bar{4}_z^{-1}|0,0,0)\)
13. \(m \quad x,0,z \quad (m_z|0,0,0)\)
14. \(m \quad 0,y,z \quad (m_z|0,0,0)\)
15. \(m' \quad x,x,z \quad (m_{xy}|0,0,0)\)
16. \(m' \quad x,x,z \quad (m_{xy}|0,0,0)\)
Continued

(1) t (1/2,1/2,1/2)  
(1 | 1/2,1/2,1/2)  

<table>
<thead>
<tr>
<th>For (1/2,1/2,1/2) + set</th>
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<tr>
<td>(1) t (1/2,1/2,1/2)</td>
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<tr>
<td>(2) 2 (0,0,1/2)</td>
</tr>
<tr>
<td>(3) 4⁺⁺ (0,0,1/2)</td>
</tr>
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<td>(4) 4⁺⁺ (0,0,1/2)</td>
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<tr>
<td>(5) 2⁺⁺ (0,1/2,0)</td>
</tr>
<tr>
<td>(6) 2⁺⁺ (1/2,0,0)</td>
</tr>
<tr>
<td>(7) 2 (1/2,1/2,0)</td>
</tr>
<tr>
<td>(8) 2 x,x + 1/2,1/4</td>
</tr>
<tr>
<td>(9) 1⁺⁺ 1/4,1/4,1/4</td>
</tr>
<tr>
<td>(10) n⁺⁺ (1/2,1/2,0)</td>
</tr>
<tr>
<td>(11) 4⁺⁺ 1/2,0,1/4</td>
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<tr>
<td>(12) 4⁺⁺ 0,1/2,1/4</td>
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<tr>
<td>(13) n⁺⁺ (1/2,1/2,1/2)</td>
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<tr>
<td>(14) n⁺⁺ (0,1/2,1/2)</td>
</tr>
<tr>
<td>(15) c⁺⁺ (0,0,1/2)</td>
</tr>
<tr>
<td>(16) n⁺⁺ (1/2,1/2,1/2)</td>
</tr>
</tbody>
</table>

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

### Positions

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<tr>
<td>32 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x⁺⁺ y⁺⁺ z⁺⁺ [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(3) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>(4) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16 n .m.</td>
<td>(5) x⁺⁺ y⁺⁺ z⁺⁺ [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(6) x⁺⁺ y⁺⁺ z⁺⁺ [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(7) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>(8) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>16 m ..m'</td>
<td>(9) x⁺⁺ y⁺⁺ z⁺⁺ [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(10) x⁺⁺ y⁺⁺ z⁺⁺ [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(11) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>(12) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>16 l m'.</td>
<td>(13) x⁺⁺ y⁺⁺ z⁺⁺ [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(14) x⁺⁺ y⁺⁺ z⁺⁺ [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(15) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>(16) y⁺⁺ x⁺⁺ z⁺⁺ [v⁺⁺ u⁺⁺ w⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>16 k .2</td>
<td>(17) x⁺⁺ x⁺⁺ 1/2,1/4 [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(18) x⁺⁺ x⁺⁺ 1/2,1/4 [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(19) x⁺⁺ x⁺⁺ 1/2,1/4 [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(20) x⁺⁺ x⁺⁺ 1/2,1/4 [u⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>8 j m'2.m.</td>
<td>(21) x⁺⁺ 1/2,0 [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(22) x⁺⁺ 1/2,0 [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(23) x⁺⁺ 1/2,0 [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(24) x⁺⁺ 1/2,0 [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>8 i m'2.m.</td>
<td>(25) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(26) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(27) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(28) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>8 h m'2.m'</td>
<td>(29) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(30) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(31) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>(32) x⁺⁺ 0⁺⁺ [0⁺⁺ v⁺⁺ w⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>8 g 2mm.</td>
<td>(33) 1/2,0,z [0⁺⁺ 0⁺⁺]</td>
<td>(34) 1/2,0,z [0⁺⁺ 0⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(35) 1/2,0,z [0⁺⁺ 0⁺⁺]</td>
<td>(36) 1/2,0,z [0⁺⁺ 0⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
<tr>
<td>8 f .2/m'</td>
<td>(37) 1/4,1/4,1/4 [0⁺⁺ 0⁺⁺]</td>
<td>(38) 1/4,1/4,1/4 [0⁺⁺ 0⁺⁺]</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(39) 1/4,1/4,1/4 [0⁺⁺ 0⁺⁺]</td>
<td>(40) 1/4,1/4,1/4 [0⁺⁺ 0⁺⁺]</td>
<td>y⁺⁺ 0⁺⁺ z⁺⁺ [0⁺⁺ u⁺⁺ 0⁺⁺]</td>
</tr>
</tbody>
</table>
Continued

| 4 | e | 4'/mm' | 0,0,z [0,0,0] | 0,0,z [0,0,0] |
| 4 | d | m2     | 0,1/2,1/4 [0,0,0] | 1/2,0,1/4 [0,0,0] |
| 4 | c | m'mm.  | 0,1/2,0 [0,0,0] | 1/2,0,0 [0,0,0] |
| 2 | b | 4'/m'mm' | 0,0,1/2 [0,0,0] |
| 2 | a | 4'/m'mm' | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

- **Along [0,0,1] p4'm'm**
  \[
a^* = \frac{a - b}{2} \quad b^* = \frac{a + b}{2}
\]
  Origin at 0,0,z
- **Along [1,0,0] c2mm1'**
  \[
a^* = b \quad b^* = c
\]
  Origin at x,0,0
- **Along [1,1,0] p2m'm'**
  \[
a^* = \frac{-a + b}{2} \quad b^* = \frac{c}{2}
\]
  Origin at x,x,0
**Origin** at center (4/m'm'm')

**Asymmetric unit**
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ y

**Symmetry Operations**

For (0,0,0) + set

1. (1) 1
   
   (1) 0,0,0

2. (2) 2 0,0,z
   
   (2) 0,0,0

3. (3) 4+ 0,0,z
   
   (4) 0,0,0

4. (4) 4- 0,0,z
   
   (4) 0,0,0

5. (5) 2 0,y,0
   
   (2) 0,0,0

6. (6) 2 x,0,0
   
   (2) 0,0,0

7. (7) 2 x,x,0
   
   (2) 0,0,0

8. (8) 2 x,x,0
   
   (2) 0,0,0

9. (9) \bar{1} 0,0,0
   
   (1) 0,0,0

10. (10) m' x,y,0

11. (11) \bar{4}+··0,0,z; 0,0,0

12. (12) \bar{4}··0,0,z; 0,0,0

13. (13) m' x,0,z

14. (14) m' 0,y,0

15. (15) m' x,x,z

16. (16) m' x,x,z
Continued

For \((1/2, 1/2, 1/2) + \) set

\[
\begin{align*}
(1) & \ t (1/2, 1/2, 1/2) \\
& (1/2, 1/2, 1/2) \\
(2) & \ 2 (0, 0, 1/2) \\
& (1/2, 1/2, 1/2) \\
(3) & \ 4^* (0, 0, 1/2) \\
& (1/2, 1/2, 1/2) \\
(4) & \ 4^* (0, 0, 1/2) \\
& (1/2, 1/2, 1/2) \\
(5) & \ 2 (0, 1/2, 0) \\
& (1/2, 1/2, 1/2) \\
& x, 1/4, 1/4 \\
(6) & \ 2 (1/2, 0, 0) \\
& (1/2, 1/2, 1/2) \\
(7) & \ 2 (1/2, 1/2, 0) \\
& (1/2, 1/2, 1/2) \\
(8) & \ 2 x, x + 1/2, 1/4 \\
& (1/2, 1/2, 1/2) \\
(9) & \ 2 y \\
& (1/2, 1/2, 1/2) \\
& x, y, 1/4 \\
(10) & \ 2 y \\
& (1/2, 1/2, 1/2) \\
& x, y, 1/4 \\
(11) & \ 4^* (1/2, 0, 1/2) \\
& (1/2, 1/2, 1/2) \\
(12) & \ 4^* (0, 0, 1/2) \\
& (1/2, 1/2, 1/2) \\
(13) & \ n' (1/2, 0, 1/2) \\
& (1/2, 1/2, 1/2) \\
& x, 1/4, z \\
(14) & \ n' (0, 1/2, 1/2) \\
& (1/2, 1/2, 1/2) \\
& x, 1/4, z \\
(15) & \ c' (0, 0, 1/2) \\
& (1/2, 1/2, 1/2) \\
(16) & \ n' (1/2, 1/2, 1/2) \\
& (1/2, 1/2, 1/2) \\
& x, x, z \\
\end{align*}
\]

Generators selected

\((1); \ t(1, 0, 0); \ t(0, 1, 0); \ t(0, 0, 1); \ t(1/2, 1/2, 1/2); \ (2); \ (3); \ (5); \ (9).\)

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry letter.

\[
\begin{array}{cccc}
32 & o & 1 & (1) x, y, z [u, v, w] \\
& & & (2) x, y, z [u, v, w] \\
& & & (3) y, x, z [v, u, w] \\
& & & (4) y, x, z [v, u, w] \\
& & & (5) x, y, z [u, v, w] \\
& & & (6) x, y, z [u, v, w] \\
& & & (7) y, x, z [v, u, w] \\
& & & (8) y, x, z [v, u, w] \\
& & & (9) x, y, z [u, v, w] \\
& & & (10) x, y, z [u, v, w] \\
& & & (11) y, x, z [v, u, w] \\
& & & (12) y, x, z [v, u, w] \\
& & & (13) x, y, z [u, v, w] \\
& & & (14) x, y, z [u, v, w] \\
& & & (15) y, x, z [v, u, w] \\
& & & (16) y, x, z [v, u, w] \\
16 & n & .m' & 0, y, z [0, v, w] \\
& & & 0, y, z [0, v, w] \\
& & & y, 0, z [0, v, w] \\
& & & y, 0, z [0, v, w] \\
16 & m & ..m' & x, x, z [u, u, w] \\
& & & x, x, z [u, u, w] \\
& & & x, x, z [u, u, w] \\
& & & x, x, z [u, u, w] \\
16 & l & m'.. & x, y, 0 [u, v, 0] \\
& & & x, y, 0 [u, v, 0] \\
& & & y, x, 0 [v, u, 0] \\
& & & y, x, 0 [v, u, 0] \\
16 & k & ..2 & x, x + 1/2, 1/4 [u, u, 0] \\
& & & x, x + 1/2, 1/4 [u, u, 0] \\
& & & x + 1/2, x, 1/4 [u, u, 0] \\
& & & x + 1/2, x, 1/4 [u, u, 0] \\
8 & j & m'2m' & x, 1/2, 0 [u, 0, 0] \\
& & & x, 1/2, 0 [u, 0, 0] \\
& & & 1/2, x, 0 [0, u, 0] \\
& & & 1/2, x, 0 [0, u, 0] \\
8 & i & m'2m' & x, 0, 0 [u, 0, 0] \\
& & & x, 0, 0 [u, 0, 0] \\
& & & 0, x, 0 [0, u, 0] \\
& & & 0, x, 0 [0, u, 0] \\
8 & h & m'.2m' & x, x, 0 [u, u, 0] \\
& & & x, x, 0 [u, u, 0] \\
& & & x, x, 0 [u, u, 0] \\
& & & x, x, 0 [u, u, 0] \\
8 & g & 2m'2m' & 0, 1/2, z [0, 0, w] \\
& & & 1/2, 0, z [0, 0, w] \\
& & & 0, 1/2, z [0, 0, w] \\
& & & 1/2, 0, z [0, 0, w] \\
8 & f & .2/m' & 1/4, 1/4, 1/4 [0, 0, 0] \\
& & & 3/4, 3/4, 1/4 [0, 0, 0] \\
& & & 3/4, 3/4, 1/4 [0, 0, 0] \\
& & & 1/4, 3/4, 1/4 [0, 0, 0]
\end{array}
\]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>Along [0,0,1] p4m'm'</th>
<th>Along [1,0,0] c2m'm'</th>
<th>Along [1,1,0] p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e</td>
<td>4m'm'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z $[0,0,w]$</td>
<td></td>
</tr>
<tr>
<td>4 d</td>
<td>4'/m'2</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4 c</td>
<td>m'm'm'</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 b</td>
<td>4/m'm'm'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a</td>
<td>4/m'm'm'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
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</tr>
</tbody>
</table>

Solutions

- Origin at 0,0,z
- Origin at 0,0,1/2
- Origin at 0,0,0
Origin at center (4/mmm)

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ y

Symmetry Operations

For (0,0,0) + set

1. (1) 1
   (1) 0,0,0

2. (2) 2 0,0,z
   (2) 2z 0,0,0

3. (3) 4⁺ 0,0,z
   (4z) 0,0,0

4. (4) 4⁻ 0,0,z
   (4z⁻¹) 0,0,0

5. (5) 2 0,y,0
   (2z) 0,0,0

6. (6) 2 x,0,0
   (2z) 0,0,0

7. (7) 2 x,x,0
   (2xy) 0,0,0

8. (8) 2 x,x,0
   (2xy) 0,0,0

9. (9) m 0,0,0
   (1) 0,0,0

10. (10) m x,y,0
    (mz) 0,0,0

11. (11) 4⁺ 0,0,z; 0,0,0
   (4z) 0,0,0

12. (12) 4⁻ 0,0,z; 0,0,0
    (4z⁻¹) 0,0,0

(13) m x,0,z
    (mz) 0,0,0

(14) m 0,y,z
    (mz) 0,0,0

(15) m x,x,z
    (mxy) 0,0,0

(16) m x,x,z
    (mxy) 0,0,0
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>o,1</td>
<td>(0,0) +</td>
</tr>
<tr>
<td>16</td>
<td>n,.m</td>
<td>(1,2,1,2,1,2)' +</td>
</tr>
<tr>
<td>16</td>
<td>m,.m</td>
<td>(0,1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>16</td>
<td>l,.m</td>
<td>(0,0,1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>8</td>
<td>m2m</td>
<td>(1/2,1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>8</td>
<td>j</td>
<td>(0,0,1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>8</td>
<td>i</td>
<td>(0,0,1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>8</td>
<td>h</td>
<td>(0,0,1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
<td>(0,0,1/2,1/2,1/2)'</td>
</tr>
<tr>
<td>8</td>
<td>f</td>
<td>(0,0,1/2,1/2,1/2)'</td>
</tr>
</tbody>
</table>

For (1/2,1/2,1/2)' + set

(1) 1' (1/2,1/2,1/2)' (2) 2' (0,0,1/2) 1/4,1/4,z (3) 4' (0,0,1/2) 0,1/2,z (4) 4' (0,0,1/2) 1/2,0,z (5) 2' (0,1/2,0) 1/4,y,1/4 (6) 2' (0,1/2,0) 1/4,y,1/4 (7) 2' (0,1/2,0) 1/4,y,1/4 (8) 2' (0,1/2,0) 1/4,y,1/4 (9) 2' (0,1/2,0) 1/4,y,1/4 (10) 2' (0,1/2,0) 1/4,y,1/4 (11) 2' (0,1/2,0) 1/4,y,1/4 (12) 2' (0,1/2,0) 1/4,y,1/4 (13) 2' (0,1/2,0) 1/4,y,1/4 (14) 2' (0,1/2,0) 1/4,y,1/4 (15) 2' (0,1/2,0) 1/4,y,1/4 (16) 2' (0,1/2,0) 1/4,y,1/4
4  e  4mm  0,0,z [0,0,0]  0,0,z [0,0,0]
4  d  4'm2'  0,1/2,1/4 [0,0,0]  1/2,0,1/4 [0,0,0]
4  c  mmm.  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]
2  b  4/mmm  0,0,1/2 [0,0,0]
2  a  4/mmm  0,0,0 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p4mm1'</td>
<td>Origin at 0,0,z</td>
<td>$a^* = (a - b)/2$ $b^* = (a + b)/2$</td>
</tr>
<tr>
<td>Along [1,0,0] c2mm1'</td>
<td>Origin at x,0,0</td>
<td>$a^* = b$ $b^* = c$</td>
</tr>
<tr>
<td>Along [1,1,0] p2mm1'</td>
<td>Origin at x,x,0</td>
<td>$a^* = (-a + b)/2$ $b^* = c/2$</td>
</tr>
</tbody>
</table>
**Origin** at center (4/m'mm)

**Asymmetric unit**
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x < y \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \(1 \quad (1|0,0,0)\)
2. \(2 \quad 0,0,z \quad (2_{z}|0,0,0)\)
3. \(4^+ \quad 0,0,z \quad (4_{z}|0,0,0)\)
4. \(4^- \quad 0,0,z \quad (4_{-z}|0,0,0)\)
5. \(2' \quad 0,y,0 \quad (2_{y}|0,0,0)'\)
6. \(2' \quad x,0,0 \quad (2_{x}|0,0,0)'\)
7. \(2' \quad x,x,0 \quad (2_{x}|0,0,0)'\)
8. \(2' \quad x,x,0 \quad (2_{-x}|0,0,0)'\)
9. \(\bar{T}^+ \quad 0,0,0 \quad (1|0,0,0)'\)
10. \(m' \quad x,y,0 \quad (m_{y}|0,0,0)'\)
11. \(\bar{4}^+ \quad 0,0,z; 0,0,0 \quad (4_{z}|0,0,0)'\)
12. \(\bar{4}^- \quad 0,0,z; 0,0,0 \quad (4_{-z}|0,0,0)'\)
13. \(m \quad x,0,z \quad (m_{z}|0,0,0)\)
14. \(m \quad 0,y,z \quad (m_{y}|0,0,0)\)
15. \(m \quad x,x,z \quad (m_{x}|0,0,0)\)
16. \(m \quad x,x,z \quad (m_{y}|0,0,0)\)
Continued

For \((1/2,1/2,1/2)^t\) + set

\[
\begin{align*}
(1) \ t'(1/2,1/2,1/2) \\
(2) \ 2'(0,0,1/2) \ 1/4,1/4,z \\
(3) \ 4^t'(0,0,1/2) \ 0,1/2,z \\
(4) \ 4^t'(0,0,1/2) \ 1/2,0,z \\
(4^t_2)(1/2,1/2,1/2)^t \\
(5) \ 2(0,1/2,0) \ 1/4,y,1/4 \\
(6) \ 2(1/2,0,0) \ x,1/4,1/4 \\
(7) \ 2(1/2,1/2,0) \ x,x,1/4 \\
(8) \ x,x+1/2,1/4 \\
(2) \ 2(1/2,1/2,1/2) \\
(2) \ 1/2,1/2,1/2 \\
(9) \ t \ 1/4,1/4,1/4 \\
(10) \ n \ (1/2,1/2,0) \ x,y,1/4 \\
(11) \ n^-1 \ 1/2,0,1/4 \ 1/2,0,1/4 \\
(12) \ n^-1 \ 0,1/2,1/4 \\
(T) \ 1/2,1/2,1/2 \\
(13) \ n' \ (1/2,0,1/2) \ x,1/4,z \\
(14) \ n' \ (0,1/2,1/2) \ 1/4,y,z \\
(15) \ c' \ (0,0,1/2) \ x+1/2,x,z \\
(16) \ n' \ (1/2,1/2,1/2) \ x,x,z \\
\end{align*}
\]

Generators selected

\((1); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).\)

**Positions**

\[
\begin{array}{cccc}
\text{Multiplicity} & \text{Wyckoff letter} & \text{Site Symmetry} & \text{Coordinates} \\
& & & (0,0,0) + (1/2,1/2,1/2)^t + \\
32 & o & 1 & x,y,z \ [u,v,w] \\
& & (2) & \bar{x},y,z \ [\bar{u},\bar{v},\bar{w}] \\
& & (3) & \bar{y},x,z \ [v,u,w] \\
& & (4) & y,x,z \ [v,\bar{u},\bar{w}] \\
& & (5) & \bar{x},y,z \ [u,v,w] \\
& & (6) & x,y,z \ [u,v,w] \\
& & (7) & y,x,z \ [v,u,w] \\
& & (8) & y,x,z \ [v,\bar{u},\bar{w}] \\
& & (9) & \bar{x},y,z \ [u,v,w] \\
& & (10) & x,y,z \ [u,v,w] \\
& & (11) & y,x,z \ [v,u,w] \\
& & (12) & y,x,z \ [v,\bar{u},\bar{w}] \\
& & (13) & \bar{x},y,z \ [u,v,w] \\
& & (14) & x,y,z \ [u,v,w] \\
& & (15) & \bar{y},x,z \ [v,u,w] \\
& & (16) & y,x,z \ [v,\bar{u},\bar{w}] \\
16 & n & \cdot.m. & 0,y,z \ [u,0,0] \\
& & (2) & \bar{y},z,0 \ [\bar{u},0,0] \\
& & (3) & y,0,z \ [0,u,0] \\
& & (4) & y,0,z \ [0,\bar{u},\bar{0}] \\
& & (5) & 0,y,z \ [u,0,0] \\
& & (6) & 0,y,z \ [u,0,0] \\
& & (7) & y,0,z \ [0,u,0] \\
& & (8) & y,0,z \ [0,\bar{u},\bar{0}] \\
16 & m & \cdot.m. & x,x,z \ [u,u,0] \\
& & (2) & x,z,0 \ [u,0,0] \\
& & (3) & x,z,0 \ [u,0,0] \\
& & (4) & x,z,0 \ [u,0,0] \\
& & (5) & x,x,z \ [u,u,0] \\
& & (6) & x,x,z \ [u,u,0] \\
& & (7) & x,x,z \ [u,u,0] \\
& & (8) & x,x,z \ [u,u,0] \\
16 & I & m'. & x,y,0 \ [u,v,0] \\
& & (2) & x,0,\bar{y} \ [\bar{u},v,0] \\
& & (3) & \bar{y},x,0 \ [\bar{v},u,0] \\
& & (4) & \bar{y},x,0 \ [\bar{v},u,0] \\
16 & k & \cdot.2 & \bar{x},x+1/2,1/4 \ [\bar{u},u,0] \\
& & (2) & \bar{x},x+1/2,1/4 \ [\bar{u},u,0] \\
& & (3) & \bar{x},x+1/2,1/4 \ [\bar{u},u,0] \\
& & (4) & \bar{x},x+1/2,1/4 \ [\bar{u},u,0] \\
& & (5) & x,x+1/2,1/4 \ [u,u,0] \\
& & (6) & x,x+1/2,1/4 \ [u,u,0] \\
& & (7) & x,x+1/2,1/4 \ [u,u,0] \\
& & (8) & x,x+1/2,1/4 \ [u,u,0] \\
8 & j & m'2.m. & x,1/2,0 \ [0,v,0] \\
& & (2) & \bar{x},x,0 \ [\bar{u},0,0] \\
& & (3) & \bar{x},x,0 \ [\bar{u},0,0] \\
& & (4) & \bar{x},x,0 \ [\bar{u},0,0] \\
8 & i & m'2.m. & x,0,0 \ [0,v,0] \\
& & (2) & x,0,0 \ [0,v,0] \\
& & (3) & x,0,0 \ [0,v,0] \\
& & (4) & x,0,0 \ [0,v,0] \\
8 & h & m'.2'm & x,x,0 \ [0,0,u] \\
& & (2) & \bar{x},x,0 \ [\bar{u},0,0] \\
& & (3) & \bar{x},x,0 \ [\bar{u},0,0] \\
& & (4) & \bar{x},x,0 \ [\bar{u},0,0] \\
8 & g & 2mm. & 0,1/2,z \ [0,0,0] \\
& & (2) & 0,1/2,z \ [0,0,0] \\
& & (3) & 0,1/2,z \ [0,0,0] \\
& & (4) & 0,1/2,z \ [0,0,0] \\
8 & f & .2/m & 1/4,1/4,1/4 \ [u,u,0] \\
& & (2) & 3/4,3/4,1/4 \ [u,u,0] \\
& & (3) & 3/4,1/4,1/4 \ [u,u,0] \\
& & (4) & 3/4,3/4,1/4 \ [u,u,0] \\
\end{array}
\]

\(139.11.1189\) - 2 - 2518
Symmetry of Special Projections

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>e</td>
<td>4mm</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>m2</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>m' mm.</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4/m' mm</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4/m' mm</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p_4. 4mm
a^* = (a - b)/2  b^* = (a + b)/2
Origin at 0,0,z

Along [1,0,0] c2mm1'
a^* = b  b^* = c
Origin at x,0,0

Along [1,1,0] p2mm1'
a^* = (-a + b)/2  b^* = c/2
Origin at x,x,0
Origin at center (4'/mm'm)

Asymmetric unit

\(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x < y\)

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \quad (1 | 0,0,0)\)
2. \(2^{'} \quad 0,0,z \quad (2_{z} | 0,0,0)'\)
3. \(4^{+-'} \quad 0,0,z \quad (4_{z} | 0,0,0)'\)
4. \(4^{+'} \quad 0,0,z \quad (4_{z} | 0,0,0)'\)
5. \(2^{'} \quad 0,y,0 \quad (2_{z} | 0,0,0)'\)
6. \(2^{'} \quad x,0,0 \quad (2_{y} | 0,0,0)'\)
7. \(2^{'} \quad x,x,0 \quad (2_{x,y} | 0,0,0)'\)
8. \(2^{'} \quad x,x,0 \quad (2_{x,y} | 0,0,0)'\)
9. \(\overline{1} \quad 0,0,0 \quad (1 | 0,0,0)\)
10. \(m \quad x,y,0 \quad (m_{z} | 0,0,0)\)
11. \(4^{+} \quad 0,0,z; 0,0,0 \quad (4_{z} | 0,0,0)'\)
12. \(4^{+} \quad 0,0,z; 0,0,0 \quad (4_{z} | 0,0,0)'\)
13. \(m' \quad x,0,z \quad (m_{z} | 0,0,0)'\)
14. \(m' \quad 0,y,z \quad (m_{y} | 0,0,0)'\)
15. \(m \quad x,x,z \quad (m_{x,y} | 0,0,0)\)
16. \(m \quad x,x,z \quad (m_{x,y} | 0,0,0)\)
Continued

For \((1/2,1/2,1/2)^*\) + set

<table>
<thead>
<tr>
<th>(1)</th>
<th>(t') ((1/2,1/2,1/2))</th>
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<tr>
<td>(1)</td>
<td>(t') ((1/2,1/2,1/2))</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>(2)</th>
<th>(2') ((0,0,1/2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2)</td>
<td>(2') ((0,0,1/2))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(3)</th>
<th>(4^*) ((0,0,1/2))</th>
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<tbody>
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<td>(3)</td>
<td>(4^*) ((0,0,1/2))</td>
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</table>

<table>
<thead>
<tr>
<th>(4)</th>
<th>(4^*) ((1/2,1/2,1/2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4)</td>
<td>(4^*) ((1/2,1/2,1/2))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(5)</th>
<th>(2) ((0,1/2,0))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5)</td>
<td>(2) ((0,1/2,0))</td>
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</table>

<table>
<thead>
<tr>
<th>(6)</th>
<th>(2) ((1/2,0,0))</th>
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<tbody>
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<td>(6)</td>
<td>(2) ((1/2,0,0))</td>
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<table>
<thead>
<tr>
<th>(7)</th>
<th>(2') ((1,2,1/2,0))</th>
</tr>
</thead>
<tbody>
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<td>(2') ((1,2,1/2,0))</td>
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</table>

<table>
<thead>
<tr>
<th>(8)</th>
<th>(2^*) ((0,1,2,1/2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(8)</td>
<td>(2^*) ((0,1,2,1/2))</td>
</tr>
</tbody>
</table>

Generators selected

(1); \(t(1,0,0);\) \(t(0,1,0);\) \(t'(1/2,1/2,1/2);\) (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry letter.</th>
<th>Coordinates</th>
<th>(0,0,0) + set</th>
<th>(1/2,1/2,1/2)^* + set</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 o 1 (x,y,z) ([u,v,w])</td>
<td>(x,y,z) ([u,v,w])</td>
<td>(x,y,z) ([v,u,w])</td>
<td>(y,x,z) ([v,u,w])</td>
</tr>
<tr>
<td>(5) (x,y,\bar{z}) ([u,v,w])</td>
<td>(x,y,\bar{z}) ([u,v,w])</td>
<td>(y,z,\bar{v}) ([v,u,w])</td>
<td>(y,z,\bar{v}) ([v,u,w])</td>
</tr>
<tr>
<td>(9) (x,\bar{y},z) ([u,v,w])</td>
<td>(x,\bar{y},z) ([u,v,w])</td>
<td>(y,\bar{z},v) ([v,u,w])</td>
<td>(y,\bar{z},v) ([v,u,w])</td>
</tr>
<tr>
<td>(13) (x,\bar{y},z) ([u,v,w])</td>
<td>(x,\bar{y},z) ([u,v,w])</td>
<td>(y,z,\bar{v}) ([v,u,w])</td>
<td>(y,z,\bar{v}) ([v,u,w])</td>
</tr>
<tr>
<td>16 n (.m'.) (0,y,z) ([0,v,w])</td>
<td>(0,y,z) ([0,v,w])</td>
<td>(y,0,z) ([v,0,w])</td>
<td>(y,0,z) ([v,0,w])</td>
</tr>
<tr>
<td>16 m (m..) (x,x,\bar{z}) ([u,u,0])</td>
<td>(x,x,\bar{z}) ([u,u,0])</td>
<td>(x,x,\bar{z}) ([u,u,0])</td>
<td>(x,x,\bar{z}) ([u,u,0])</td>
</tr>
<tr>
<td>16 l (m..) (x,y,0) ([0,0,w])</td>
<td>(x,y,0) ([0,0,w])</td>
<td>(y,x,0) ([0,0,w])</td>
<td>(y,x,0) ([0,0,w])</td>
</tr>
<tr>
<td>16 k (m2m'.) (x,x+1/2,1/4) ([u,u,w])</td>
<td>(x,x+1/2,1/4) ([u,u,w])</td>
<td>(x,x+1/2,1/4) ([u,u,w])</td>
<td>(x,x+1/2,1/4) ([u,u,w])</td>
</tr>
<tr>
<td>8 j (m2m'.) (x,1/2,0) ([0,0,w])</td>
<td>(x,1/2,0) ([0,0,w])</td>
<td>(1/2,x,0) ([0,0,w])</td>
<td>(1/2,x,0) ([0,0,w])</td>
</tr>
<tr>
<td>8 i (m2m'.) (x,0,0) ([0,0,w])</td>
<td>(x,0,0) ([0,0,w])</td>
<td>(0,x,0) ([0,0,w])</td>
<td>(0,x,0) ([0,0,w])</td>
</tr>
<tr>
<td>8 h (m2m) (x,x,0) ([0,0,0])</td>
<td>(x,x,0) ([0,0,0])</td>
<td>(x,x,0) ([0,0,0])</td>
<td>(x,x,0) ([0,0,0])</td>
</tr>
<tr>
<td>8 g (2m'.) (0,1/2,0) ([0,0,w])</td>
<td>(0,1/2,0) ([0,0,w])</td>
<td>(0,1/2,0) ([0,0,w])</td>
<td>(0,1/2,0) ([0,0,w])</td>
</tr>
<tr>
<td>8 f (.2'm) (1/4,1/4,1/4) ([0,0,0])</td>
<td>(1/4,1/4,1/4) ([0,0,0])</td>
<td>(1/4,3/4,1/4) ([0,0,0])</td>
<td>(1/4,3/4,1/4) ([0,0,0])</td>
</tr>
<tr>
<td>4 e</td>
<td>4’m’m</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,ζ [0,0,0]</td>
</tr>
<tr>
<td>-----</td>
<td>-------</td>
<td>---------------</td>
<td>---------------</td>
</tr>
<tr>
<td>4 d</td>
<td>4’m’2’</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>1/2,0,1/4 [0,0,ν]</td>
</tr>
<tr>
<td>4 c</td>
<td>mm’m’</td>
<td>0,1/2,0 [0,0,w]</td>
<td>1/2,0,0 [0,0,ν]</td>
</tr>
<tr>
<td>2 b</td>
<td>4’/mm’</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a</td>
<td>4’/mm’</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1’</th>
<th>Along [1,0,0] c2’mm’</th>
<th>Along [1,1,0] p2mm1’</th>
</tr>
</thead>
<tbody>
<tr>
<td>a’ = (a - b)/2</td>
<td>a’ = -c</td>
<td>a’ = (-a + b)/2</td>
</tr>
<tr>
<td>b’ = (a + b)/2</td>
<td>b’ = b</td>
<td>b’ = c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,ζ | Origin at x,0,0 | Origin at x,x,0
Origin at center (4'/mmm')

Asymmetric unit  
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x < y \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \quad (1|0,0,0) \)
2. \(2 \quad 0,0,z \quad (2_z|0,0,0) \)
3. \(4'^+ \quad 0,0,z \quad (4_z|0,0,0)' \)
4. \(4' \quad 0,0,z \quad (4_z^{-1}|0,0,0)' \)
5. \(2 \quad 0,y,0 \quad (2_y|0,0,0) \)
6. \(2 \quad x,0,0 \quad (2_x|0,0,0) \)
7. \(2' \quad x,x,0 \quad (2_{xy}|0,0,0)' \)
8. \(2' \quad x,x,0 \quad (2_{xy}|0,0,0)' \)
9. \(1 \quad 0,0,0 \quad (1|0,0,0) \)
10. \(m \quad x,y,0 \quad (m_{yz}|0,0,0) \)
11. \(4' \quad 0,0,z; 0,0,0 \quad (4_z|0,0,0)' \)
12. \(4' \quad 0,0,z; 0,0,0 \quad (4_z^{-1}|0,0,0)' \)
13. \(m \quad x,0,z \quad (m_{y}|0,0,0) \)
14. \(m \quad 0,y,z \quad (m_{x}|0,0,0) \)
15. \(m' \quad x,x,z \quad (m_{xy}|0,0,0)' \)
16. \(m' \quad x,x,z \quad (m_{xy}|0,0,0)' \)
### Generators selected
1: \((1,0,0)\); 2: \((0,1,0)\); 3: \((0,0,1)\); 4: \((1/2,1/2,1/2)\); 5: \((1/2,1/2,1/2)\); 6: \((1/2,1/2,1/2)\); 7: \((1/2,1/2,1/2)\); 8: \((1/2,1/2,1/2)\); 9: \((1/2,1/2,1/2)\); 10: \((1/2,1/2,1/2)\); 11: \((1/2,1/2,1/2)\); 12: \((1/2,1/2,1/2)\); 13: \((1/2,1/2,1/2)\); 14: \((1/2,1/2,1/2)\); 15: \((1/2,1/2,1/2)\); 16: \((1/2,1/2,1/2)\); 17: \((1/2,1/2,1/2)\);

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 0 1</td>
<td>((x,y,z))</td>
<td>(u,v,w)</td>
<td>((0,0,0))</td>
<td>((1/2,1/2,1/2)) + set</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>((x,y,z))</td>
<td>(u,v,w)</td>
<td>((0,0,0))</td>
<td>((1/2,1/2,1/2)) + set</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16 m ..m'</td>
<td>(x,x,z)</td>
<td>(u,u,w)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>16 m ..m'</td>
<td>(x,x,z)</td>
<td>(u,u,w)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>16 l ..m'</td>
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<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>16 l ..m'</td>
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<td>((1/2,1/2,1/2)) + set</td>
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</tr>
<tr>
<td>16 k ..2</td>
<td>(x,x+1/2,1/4)</td>
<td>(u,u,0)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>8 j m2m.</td>
<td>(x,1/2,0)</td>
<td>(0,0,0)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>8 i m2m.</td>
<td>(x,0,0)</td>
<td>(0,0,0)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>8 h m.2'm'</td>
<td>(x,x,0)</td>
<td>(0,0,0)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>8 g 2mm.</td>
<td>(1/2,0,2)</td>
<td>(0,0,0)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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<tr>
<td>8 f ..2/m'</td>
<td>(1/4,1/4,1/4)</td>
<td>(0,0,0)</td>
<td>((1/2,0,1/2))</td>
<td>((1/2,1/2,1/2)) + set</td>
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</table>
### Symmetry of Special Projections

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<tbody>
<tr>
<td>4</td>
<td>e</td>
<td>4'\text{mm}'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,\overline{z} [0,0,0]</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>4</td>
<td>d</td>
<td>\text{\overline{4}m2}</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
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</tr>
<tr>
<td>4</td>
<td>c</td>
<td>\text{mmm}</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4'/\text{mmm}'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
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</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4'/\text{mmm}'</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

**Origin at 0,0,z**

**Origin at x,0,0**

**Origin at x,x,1/4**

**Along [0,0,1] p4mm1'**

\[ a^* = \frac{a - b}{2} \]

\[ b^* = \frac{a + b}{2} \]

**Along [1,0,0] c2mm1'**

\[ a^* = b \]

\[ b^* = c \]

**Along [1,1,0] p_{2a} 2m'm'**

\[ a^* = -c/2 \]

\[ b^* = \frac{-a + b}{2} \]
I₄/m'm'm 139.14.1192
4/mmm1' 139.14.1192
I₄/m'2/m'2/m Tetragonal

Origin at center (4'/m'm'm)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ y

Symmetry Operations
For (0,0,0) + set

(1) 1 (1|0,0,0)
(5) 2 0,y,0 (2|0,0,0)
(9) 1' 0,0,0 (1|0,0,0)'
(13) m' x,0,z (m'|0,0,0)'

(2) 2 0,0,z (2z|0,0,0)
(6) 2 x,0,0 (2x|0,0,0)
(10) m' x,y,0 (m'|0,0,0)'
(14) m' 0,y,z (m'|0,0,0)'

(3) 4' 0,0,z (4z|0,0,0)'
(7) 2' x,x,0 (2x|0,0,0)'
(11) 4' 0,0,z; 0,0,0 (4z|0,0,0)
(15) m x,x,z (m|0,0,0)

(4) 4' 0,0,z (4z|0,0,0)'
(8) 2' x,x,0 (2x|0,0,0)'
(12) 4' 0,0,z; 0,0,0 (4z|0,0,0)
(16) m x,x,z (m|0,0,0)
Continued

For (1/2,1/2,1/2') + set

(1) t' (1/2,1/2,1/2)  (2) 2' (0,0,1/2)  1/4,1/4,z  (3) 4' (0,0,1/2)  0,1/2,z  (4) 4' (0,0,1/2)  1/2,0,z
(1 | 1/2,1/2,1/2')  (2 | 1/2,1/2,1/2')  (4 | 1/2,1/2,1/2')

(5) 2' (0,1/2,0)  1/4,y,1/4  (6) 2' (1/2,0,0)  x,1/4,1/4  (7) 2 (1/2,1/2,0)  x,x,1/4
(2 | 1/2,1/2,1/2')  (2 | 1/2,1/2,1/2')  (2 | 1/2,1/2,1/2')

(9) \( \frac{1}{2} \) 1/4,1/4,1/4  (10) n (1/2,1/2,0)  x,y,z
\( \frac{1}{2} \) 1/2,1/2,1/2'  \( \frac{1}{2} \) 1/2,1/2,1/2'

(13) n (1/2,0,1/2)  x,1/4,z  (14) n (0,1/2,1/2)  1/4,y,z  (15) c' (0,0,1/2)  x+1/2,x',z
(\( \frac{1}{2} \) 1/2,1/2,1/2)  (\( \frac{1}{2} \) 1/2,1/2,1/2')  (\( \frac{1}{2} \) 1/2,1/2,1/2')

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2') +</td>
</tr>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2') +</td>
</tr>
<tr>
<td>32 o 1</td>
<td>32 o 1</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x',y',z [u',v',w]</td>
</tr>
<tr>
<td>(3) y,x,z [v,u,w]</td>
<td>(4) y,x',z [v',u,w]</td>
</tr>
<tr>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x',y',z [u',v',w]</td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) y,x',z [v',u,w]</td>
</tr>
<tr>
<td>(9) x,y,z [u,v,w]</td>
<td>(10) x',y',z [u',v',w]</td>
</tr>
<tr>
<td>(11) y,x,z [v,u,w]</td>
<td>(12) y,x',z [v',u,w]</td>
</tr>
<tr>
<td>(13) x,y,z [u,v,w]</td>
<td>(14) x',y',z [u',v',w]</td>
</tr>
<tr>
<td>(15) y,x,z [v,u,w]</td>
<td>(16) y,x,z [v',u,w]</td>
</tr>
<tr>
<td>16 n ..m'..</td>
<td>16 n ..m'..</td>
</tr>
<tr>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>0,y,z [0,v,w]</td>
<td>0,y,z [0,v,w]</td>
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<tr>
<td>16 m ..m</td>
<td>16 m ..m</td>
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<tr>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
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<tr>
<td>x,x,z [u,u,0]</td>
<td>x,x,z [u,u,0]</td>
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<tr>
<td>16 l ..m'..</td>
<td>16 l ..m'..</td>
</tr>
<tr>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
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<tr>
<td>x,y,0 [u,v,0]</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>16 k ..2</td>
<td>16 k ..2</td>
</tr>
<tr>
<td>x,x+1/2,1/4 [u,u,0]</td>
<td>x,x+1/2,1/4 [u,u,0]</td>
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<tr>
<td>x,x+1/2,1/4 [u,u,0]</td>
<td>x,x+1/2,1/4 [u,u,0]</td>
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<tr>
<td>8 j m'2m'..</td>
<td>8 j m'2m'..</td>
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<tr>
<td>x,1/2,0 [u,u,0]</td>
<td>x,1/2,0 [u,u,0]</td>
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<td>x,1/2,0 [u,u,0]</td>
<td>x,1/2,0 [u,u,0]</td>
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<tr>
<td>8 i m'2m'..</td>
<td>8 i m'2m'..</td>
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<td>x,0,0 [u,u,0]</td>
<td>x,0,0 [u,u,0]</td>
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<td>x,0,0 [u,u,0]</td>
<td>x,0,0 [u,u,0]</td>
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<tr>
<td>8 h m'.2m</td>
<td>8 h m'.2m</td>
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<tr>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
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<tr>
<td>x,x,0 [u,u,0]</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>8 g 2m'm'..</td>
<td>8 g 2m'm'..</td>
</tr>
<tr>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>0,1/2,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>8 f ..2/m</td>
<td>8 f ..2/m</td>
</tr>
<tr>
<td>1/4,1/4,1/4 [u,u,0]</td>
<td>1/4,1/4,1/4 [u,u,0]</td>
</tr>
<tr>
<td>1/4,1/4,1/4 [u,u,0]</td>
<td>1/4,1/4,1/4 [u,u,0]</td>
</tr>
</tbody>
</table>

139.14.1192 - 2 - 2527
4  e  4' m'm  0,0,z [0,0,0]  0,0,z [0,0,0]
4  d  4' m'2  0,1/2,1/4 [0,0,0]  1/2,0,1/4 [0,0,0]
4  c  m'm'm'  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]
2  b  4'/m'm'm  0,0,1/2 [0,0,0]
2  a  4'/m'm'm  0,0,0 [0,0,0]

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Symmetry</th>
<th>Origin</th>
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<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p, 4'mm'</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>c, 2m'm'</td>
<td>x,0,0</td>
</tr>
<tr>
<td>a* = b</td>
<td>b* = c</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p2mm1'</td>
<td>x,x,0</td>
</tr>
<tr>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin at center (4/mm'm')

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x \leq y$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
   \[1(0,0,0)\]

2. $2 \cdot 0,0,z$
   \[2(2z,0,0,0)\]

3. $4^+ \cdot 0,0,z$
   \[4^+(4z,0,0,0)\]

4. $4^- \cdot 0,0,z$
   \[4^-(4z^{-1},0,0,0)\]

5. $2' \cdot 0,y,0$
   \[(2y,0,0,0)\]

6. $2' \cdot x,0,0$
   \[(2x,0,0,0)\]

7. $2' \cdot x,x,0$
   \[(2x,0,0,0)\]

8. $2' \cdot x,x,0$
   \[(2x,0,0,0)\]

9. $m' \cdot x,0,z$
   \[(m_x,0,0,0)\]

10. $m' \cdot y,z$
    \[(m_y,0,0,0)\]

11. $m' \cdot x,x,z$
    \[(m_{xy},0,0,0)\]

12. $m' \cdot x,x,z$
    \[(m_{xy},0,0,0)\]

13. $m' \cdot x,0,z$
    \[(m_x,0,0,0)\]

14. $m' \cdot y,z$
    \[(m_y,0,0,0)\]

15. $m' \cdot x,x,z$
    \[(m_{xy},0,0,0)\]

16. $m' \cdot x,x,z$
    \[(m_{xy},0,0,0)\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<tr>
<td>32</td>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2') +</td>
</tr>
<tr>
<td>16</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td>16</td>
<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
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<td>(9) x,y,z [u,v,w]</td>
<td>(10) x,y,z [u,v,w]</td>
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<td>(13) x,y,z [u,v,w]</td>
<td>(14) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16</td>
<td>(17) x,y,z [u,v,w]</td>
<td>(18) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>8</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<td>(5) x,y,z [u,v,w]</td>
<td>(6) x,y,z [u,v,w]</td>
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<td>(10) x,y,z [u,v,w]</td>
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<td>(13) x,y,z [u,v,w]</td>
<td>(14) x,y,z [u,v,w]</td>
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<tr>
<td>8</td>
<td>(17) x,y,z [u,v,w]</td>
<td>(18) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

Continued

For (1/2,1/2,1/2') + set

(1) t' (1/2,1/2,1/2)
(2) 2' (0,0,1/2) 1/4,1/4,z
(3) 4' (0,0,1/2) 0,1/2,z
(4) 4' (0,0,1/2) 1/2,0,z
(5) 2 (0,1/2,0) 1/4,1/4,z
(6) 2 (1/2,0,0) 1/2,0,1/4
(7) 2 (1/2,1/2,0) 1/2,0,1/4
(8) 2 (1/2,1/2,0) 1/2,0,1/4
(9) 1' 1/2,1/2,1/2')
(10) n' (1/2,1/2,0) x,1/4,1/4
(11) 4' (1/2,0,1/2) 1/2,0,1/4
(12) 4' (1/2,1/2,0) 1/2,0,1/4
(13) n (1/2,0,1/2) x,1/4,z
(14) n (0,1/2,1/2) 1/4,y,z
(15) c (0,0,1/2) x+1/2,x,z
(16) n (1/2,1/2,1/2) x,x,z
(17) n (0,1/2,1/2) 1/4,y,z
(18) n (1/2,1/2,1/2) x,x,z

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).
4 e 4m'm' 0,0,z [0,0,w] 0,0,z [0,0,w]
4 d 4'm'2 0,1/2,1/4 [0,0,0] 1/2,0,1/4 [0,0,0]
4 c mm'm'. 0,1/2,0 [0,0,w] 1/2,0,0 [0,0,w]
2 b 4/mm'm' 0,0,1/2 [0,0,w]
2 a 4/mm'm' 0,0,0 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p4mm1'
\[a^* = (a - b)/2 \quad b^* = (a + b)/2\]
Origin at 0,0,z

Along [1,0,0] c_p, 2'mm'
\[a^* = -c \quad b^* = b\]
Origin at x,0,0

Along [1,1,0] p_2a, 2m'm'
\[a^* = -c/2 \quad b^* = (-a + b)/2\]
Origin at x,x,1/4
**Origin** at center (4/m'nm')

**Asymmetric unit**

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4} \; \text{and} \; x \leq y \]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>1</td>
<td>((1</td>
</tr>
<tr>
<td>(2)</td>
<td>2' 0,0,z</td>
<td>((2_z</td>
</tr>
<tr>
<td>(3)</td>
<td>4' 0,0,z</td>
<td>((4_z</td>
</tr>
<tr>
<td>(4)</td>
<td>4' -1 0,0,z</td>
<td>((4_{z'}</td>
</tr>
<tr>
<td>(5)</td>
<td>2' 0,y,0</td>
<td>((2_y</td>
</tr>
<tr>
<td>(6)</td>
<td>2' x,0,0</td>
<td>((2_x</td>
</tr>
<tr>
<td>(7)</td>
<td>2 (x,x,0)</td>
<td>((2_{xx}</td>
</tr>
<tr>
<td>(8)</td>
<td>2 (x,\bar{x},0)</td>
<td>((2_{x\bar{x}}</td>
</tr>
<tr>
<td>(9)</td>
<td>(\bar{1}) 0,0,0</td>
<td>((1'</td>
</tr>
<tr>
<td>(10)</td>
<td>(m) x,y,0</td>
<td>((m_z</td>
</tr>
<tr>
<td>(11)</td>
<td>(\bar{4}) 0,0,z</td>
<td>((\bar{4}_z</td>
</tr>
<tr>
<td>(12)</td>
<td>(\bar{4}) -1 0,0,z</td>
<td>((\bar{4}_{z'}</td>
</tr>
<tr>
<td>(13)</td>
<td>m x,0,z</td>
<td>((m_x</td>
</tr>
<tr>
<td>(14)</td>
<td>m 0,y,z</td>
<td>((m_y</td>
</tr>
<tr>
<td>(15)</td>
<td>m' (x,x,z)</td>
<td>((m_{xx}</td>
</tr>
<tr>
<td>(16)</td>
<td>m' (x,\bar{x},z)</td>
<td>((m_{x\bar{x}}</td>
</tr>
</tbody>
</table>
For \((1/2,1/2,1/2)'+\) + set

\[
\begin{align*}
(1) \ t' (1/2,1/2,1/2)
(2) \ 2' (0,0,1/2) \\
(3) \ 4^+ (0,0,1/2)
(4) \ 4^+ (0,0,1/2)
\end{align*}
\]

\[
\begin{align*}
(5) \ 2 (0,1/2,0) \\
(6) \ 2 (1/2,0,0) \\
(7) \ 2' (1/2,1/2,0)
(8) \ 2' x,x+1/2,1/4
(2,1/2,1/2)'
\end{align*}
\]

\[
\begin{align*}
(9) \ \bar{1} \ 1/4,1/4,1/4 \\
(10) \ n (1/2,1/2,0) \\
(11) \ 4^+ \ 1/2,0,z; 1/2,0,1/4
(2,1/2,1/2)'
(4,z) \ 1/2,1/2,1/2)'
\end{align*}
\]

\[
\begin{align*}
(13) \ n' (1/2,0,1/2) \\
(14) \ n' (0,1/2,1/2) \\
(15) \ c (0,0,1/2) \\
(16) \ n (1/2,1/2,1/2)
\end{align*}
\]

\[
\begin{align*}
(12) \ 4^- \ 0,1/2,z; 0,1/2,1/4
(4,z) \ 1/2,1/2,1/2)'
\end{align*}
\]

\[
\begin{align*}
(13) \ x,y,z \\
(14) \ x,y,z \\
(15) \ x,y,z \\
(16) \ y,x,z
\end{align*}
\]

\[
\begin{align*}
(13) \ x,y,z \\
(14) \ x,y,z \\
(15) \ y,x,z \\
(16) \ y,x,z
\end{align*}
\]

\[
\begin{align*}
(13) \ x,y,z \\
(14) \ x,y,z \\
(15) \ y,x,z \\
(16) \ y,x,z
\end{align*}
\]

Generators selected (1); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry, Coordinates

\[
\begin{align*}
(0,0,0) + & \quad (1/2,1/2,1/2)'+ \\
32 & \ o \ 1 \\
(1) \ x,y,z [u,v,w] & \quad (2) \ x,y,z [u,v,w] \\
(5) \ x,y,z [u,v,w] & \quad (6) \ x,y,z [u,v,w] \\
(9) \ x,y,z [u,v,w] & \quad (10) \ x,y,z [u,v,w] \\
(13) \ x,y,z [u,v,w] & \quad (14) \ x,y,z [u,v,w] \\
16 & \ n \ .m. \\
(0,y,z [u,0,0] & \quad (1/y,z [0,0,0] \\
0,y,z [u,0,0] & \quad 0,y,z [0,0,0] \\
0,y,z [u,0,0] & \quad 0,y,z [0,0,0] \\
0,y,z [u,0,0] & \quad 0,y,z [0,0,0] \\
16 & \ m \ .m' \\
(x,x,z [u,u,w] & \quad (x,x,z [u,u,w] \\
(x,x,z [u,u,w] & \quad (x,x,z [u,u,w] \\
(x,x,z [u,u,w] & \quad (x,x,z [u,u,w] \\
16 & \ l \ .m' \\
(x,y,0 [u,v,0] & \quad (x,y,0 [u,v,0] \\
(x,y,0 [u,v,0] & \quad (x,y,0 [u,v,0] \\
(x,y,0 [u,v,0] & \quad (x,y,0 [u,v,0] \\
16 & \ k \ .2' \\
(x,x+1/2,1/4 [u,u,w] & \quad (x,x+1/2,1/4 [u,u,w] \\
(x,x+1/2,1/4 [u,u,w] & \quad (x,x+1/2,1/4 [u,u,w] \\
(x,x+1/2,1/4 [u,u,w] & \quad (x,x+1/2,1/4 [u,u,w] \\
8 & \ j \ m'2.m. \\
(x,1/2,0 [u,v,0] & \quad (x,1/2,0 [u,v,0] \\
(x,1/2,0 [u,v,0] & \quad (x,1/2,0 [u,v,0] \\
(x,1/2,0 [u,v,0] & \quad (x,1/2,0 [u,v,0] \\
8 & \ i \ m'2.m. \\
(x,0,0 [v,0,0] & \quad (x,0,0 [v,0,0] \\
(x,0,0 [v,0,0] & \quad (x,0,0 [v,0,0] \\
(x,0,0 [v,0,0] & \quad (x,0,0 [v,0,0] \\
8 & \ h \ m'.2m' \\
(x,x,0 [u,u,0] & \quad (x,x,0 [u,u,0] \\
(x,x,0 [u,u,0] & \quad (x,x,0 [u,u,0] \\
(x,x,0 [u,u,0] & \quad (x,x,0 [u,u,0] \\
8 & \ g \ 2mm. \\
(0,1/2,z [0,0,0] & \quad (0,1/2,z [0,0,0] \\
(0,1/2,z [0,0,0] & \quad (0,1/2,z [0,0,0] \\
(0,1/2,z [0,0,0] & \quad (0,1/2,z [0,0,0] \\
8 & \ f \ .2'/m' \\
3/4,1/4,1/4 [u,u,0] & \quad 3/4,1/4,1/4 [u,u,0] \\
3/4,1/4,1/4 [u,u,0] & \quad 3/4,1/4,1/4 [u,u,0] \\
3/4,1/4,1/4 [u,u,0] & \quad 3/4,1/4,1/4 [u,u,0]
\end{align*}
\]

139.16.1194 - 2 - 2533
Symmetry of Special Projections

Along \([0,0,1]\) \(p_{\rho}, 4'm'm\)  
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along \([1,0,0]\) \(c2mm1'\)  
\[ a^* = b \quad b^* = c \]
Origin at x,0,0

Along \([1,1,0]\) \(p_{2\alpha}, 2m'm'\)  
\[ a^* = -c/2 \quad b^* = (a + b)/2 \]
Origin at x,x,0
Origin at center (4/m'm'm')

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ y

Symmetry Operations

For (0,0,0) + set

(1) 1
    (1|0,0,0)

(5) 2  0,y,0
    (2|0,0,0)

(9) 1' 0,0,0
    (1'|0,0,0)'

(13) m'  x,0,z
    (m'|0,0,0)'

(2) 2  0,0,z
    (2z|0,0,0)

(6) 2  x,0,0
    (2z|0,0,0)

(10) m'  x,y,0
    (m|0,0,0)'

(11) 4' 0,0,z
    (4z|0,0,0)

(15) m'  x,x,z
    (mxy|0,0,0)'

(3) 4' 0,0,z
    (4z|0,0,0)

(7) 2  x,x,0
    (2xy|0,0,0)

(11) 4' 0,0,z
    (4z|0,0,0)'

(15) m'  x,x,z
    (mxy|0,0,0)'

(4) 4' 0,0,z
    (4z|0,0,0)

(8) 2  x,x,0
    (2xy|0,0,0)

(12) 4' 0,0,z
    (4z|0,0,0)'

(16) m'  x,x,z
    (mxy|0,0,0)'
Continued

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)
   1/4,1/4,z
(1,1/2,1/2,1/2)

(2) 2' (0,0,1/2)
   1/4,1/4,z
(2,1/2,1/2,1/2)

(3) 4' (0,0,1/2)
   0,1/2,z
(4,1/2,1/2,1/2)

(4) 4' (0,0,1/2)
   1/2,0,z
(4,1/2,1/2,1/2)

(5) 2' (0,1/2,0)
   1/4,y,1/4
(2,1/2,1/2,1/2)

(6) 2' (1/2,1/2,0)
   x,1/4,1/4
(2,1/2,1/2,1/2)

(7) 2' (1/2,1/2,0)
   x,x,1/4
(2,1/2,1/2,1/2)

(8) 2' x,x+1/2,1/4
(2,1/2,1/2,1/2)

(9) T 1/4,1/4,1/4
(1/2,1/2,1/2)

(10) n' (1/2,1/2,1/2)
   x,x,z
(1/2,1/2,1/2)

(11) 4' (0,0,1/2)
   1/2,0,z
(4,1/2,1/2,1/2)

(12) 4' 1/2,0,z; 1/2,0,1/4
(4,1/2,1/2,1/2)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>32 o 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>16 n .m'</td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>0,y,z [0,v,w]</td>
</tr>
<tr>
<td>16 m .m'</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>16 l .m'</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td>16 k .2'</td>
<td>x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x+1/2,1/4 [u,u,w]</td>
</tr>
<tr>
<td>8 j .m'2m'</td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>8 i .m'2m'</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>8 h .m'2m'</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>8 g 2m'm'</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 f .2'm'</td>
<td>1/4,1/4,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>3/4,3/4,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>1/4,3/4,1/4 [u,u,0]</td>
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</tbody>
</table>

139.17.1195 - 2 - 2536
### Symmetry of Special Projections

<p>| | | | | | |</p>
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</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>e</td>
<td>4/m'm'm'</td>
<td>0,0,z</td>
<td>[0,0,w]</td>
<td>0,0,z</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>4/m'2'</td>
<td>0,1/2,1/4</td>
<td>[0,0,w]</td>
<td>1/2,0,1/4</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>m'm'm'.</td>
<td>0,1/2,0</td>
<td>[0,0,0]</td>
<td>1/2,0,0</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>4/m'm'm'</td>
<td>0,0,1/2</td>
<td>[0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>4/m'm'm'</td>
<td>0,0,0</td>
<td>[0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]** p4/m'm'
  - \(a^* = \frac{a - b}{2}\)
  - \(b^* = \frac{a + b}{2}\)
  - Origin at 0,0,z

- **Along [1,0,0]** c_p 2m'm'
  - \(a^* = b\)
  - \(b^* = c\)
  - Origin at x,0,0

- **Along [1,1,0]** p_2a_2 2m'm'
  - \(a^* = -\frac{c}{2}\)
  - \(b^* = -\frac{a + b}{2}\)
  - Origin at x,x,0
### Origin

Origin at center (4/m) at 4/mc₂/c

### Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad y \leq \frac{1}{2} - x \]

### Symmetry Operations

For \((0,0,0) + \) set

<table>
<thead>
<tr>
<th>Index</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>4⁺⁺ 0,0,z</td>
</tr>
<tr>
<td>4</td>
<td>4⁻⁻ 0,0,z</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
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<td>2</td>
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<tr>
<td>9</td>
<td>1</td>
</tr>
<tr>
<td>10</td>
<td>m</td>
</tr>
<tr>
<td>11</td>
<td>4⁺⁺ 0,0,z</td>
</tr>
<tr>
<td>12</td>
<td>4⁻⁻ 0,0,z</td>
</tr>
<tr>
<td>13</td>
<td>c</td>
</tr>
<tr>
<td>14</td>
<td>c</td>
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<tr>
<td>15</td>
<td>c</td>
</tr>
<tr>
<td>16</td>
<td>c</td>
</tr>
</tbody>
</table>

### Diagram

[Diagram showing the crystal structure with symmetry operations indicated]
Continued

For $(1/2,1/2,1/2) + \text{ set}$

<table>
<thead>
<tr>
<th>(1) t $(1/2,1/2,1/2)$</th>
<th>(2) 2 $(0,0,1/2)$</th>
<th>1/4,1/4,z</th>
<th>(3) $4^+$ $(0,0,1/2)$</th>
<th>0,1/2,z</th>
<th>(4) $4^-$ $(0,0,1/2)$</th>
<th>1/2,0,z</th>
<th>(4) $z^{-1}$</th>
<th>1/2,1,2,1/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1/2,1/2,1/2)$</td>
<td>$(2,1/2,1/2,1/2)$</td>
<td></td>
<td>$(3,1/2,1/2,1/2)$</td>
<td></td>
<td>$(4,1/2,1/2,1/2)$</td>
<td></td>
<td>$(4,1/2,1/2,1/2)$</td>
<td></td>
</tr>
</tbody>
</table>

| (5) 2 $(0,1/2,0)$     | 1/4,y,0         |          | (6) 2 $(1/2,0,0)$ | x,1/4,0  | (7) 2 $(1/2,1/2,0)$ | x,x,0   | (8) $2 \bar{x},\bar{x}+1/2,0$ |          |
| $(2,1/2,1/2,0)$      | $(2,1/2,1/2,0)$ |          | $(2,1/2,1/2,0)$ |          | $(2,1/2,1/2,0)$ |          | $(2,1/2,1/2,0)$ |          |

| (9) $\Gamma$ 1/4,1,4/4 | (10) n $(1/2,1/2,0)$ | x,y,1/4  | (11) $4^+$ 1/2,0,z | 1/2,0,1/4 | (12) $4^-$ 0,1/2,z | 0,1/2,1/4 | (4) $z^{-1}$ | 1/2,1,2,1/2 |
| $1/2,1,2,1/2$       | $(m,1/2,1,2,1/2)$|          | $(4,1/2,1,2,1/2)$|          | $(4,1/2,1,2,1/2)$|          | $(4,1/2,1,2,1/2)$|          |

| (13) a $(1/2,0,0)$   | x,1/4,z         |          | (14) b $(0,1/2,0)$ | 1/4,y,z  | (15) m x+1/2, x,z |          | (16) g $(1/2,1/2,0)$ | x,x,z   |
| $(m,1/2,1,2,0)$     | $(m,1/2,1,2,0)$ |          | $(m,1/2,1,2,0)$ |          | $(m,1/2,1,2,0)$ |          | $(m,1/2,1,2,0)$ |          |

**Generators selected**

$(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1,2,1/2); (2); (3); (5); (9).$

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>m 1</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>l m..</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>k m..</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>j .2</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>i .2</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>h m.2m</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>g 2.mm</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>f 4..</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>e .2/m</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>d m.mm</td>
<td></td>
</tr>
</tbody>
</table>

**Coordinates**

<table>
<thead>
<tr>
<th></th>
<th>(0,0,0) +</th>
<th>(1/2,1/2,1/2) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(2) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(3) y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(4) y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(6) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(8) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(9) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(10) x,y,z [u,v,w]</td>
<td>x,y,z [u,v,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(11) y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(12) y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
<td>y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(13) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(14) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(15) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(16) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(17) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(18) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(19) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(20) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(21) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(22) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(23) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(24) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(25) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(26) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(27) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(28) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(29) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(30) x,y,z+1/2 [u,v,w]</td>
<td>x,y,z+1/2 [u,v,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(31) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(32) y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
<td>y,x,z+1/2 [v,u,w]</td>
</tr>
</tbody>
</table>

**Wyckoff letter, Site Symmetry.**
Continued

| 4 | c | 4/m.. | 0,0,0 [0,0,w] | 0,0,1/2 [0,0,w] |
| 4 | b | 42m  | 0,1/2,1/4 [0,0,0] | 1/2,0,1/4 [0,0,0] |
| 4 | a | 422  | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,0,0] p_a2mm  
\[ a^* = b/2 \quad b^* = c/2 \]
Origin at x,1/4,0

Along [1,1,0] p2mm1'  
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x,0
**Origin** at center (4/m1') at 4/mc21/c1'

**Asymmetric unit**

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/4; \quad y < 1/2 - x \]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \((1) 1\)
   
2. \((2) z, 0, 0, 0\)

3. \((3) 4^+ z, 0, 0, 0\)

4. \((4) 4^- z, 0, 0, 0\)

5. \((5) 2 z, 0, 0, 0\)

6. \((6) 2 z, 0, 0, 0\)

7. \((7) 2 z, 0, 0, 0\)

8. \((8) 2 z, 0, 0, 0\)

9. \((9) 2 y, 0, 0, 0\)

10. \((10) 2 y, 0, 0, 0\)

11. \((11) 2 y, 0, 0, 0\)

12. \((12) 2 y, 0, 0, 0\)

13. \((13) c x, 0, 0, 0\)

14. \((14) c x, 0, 0, 0\)

15. \((15) c x, 0, 0, 0\)

16. \((16) c x, 0, 0, 0\)
Continued

For \((1/2,1/2,1/2) +\) set

\[
\begin{align*}
(1) & \ t (1/2,1/2,1/2) \\
(1) & \ t (1/2,1/2,1/2) \\
(2) & \ 2 (0,0,1/2) \ 1/4,1/4,z \\
(2) & \ 2 (0,0,1/2) \ 1/4,1/4,z \\
(3) & \ 4^+ (0,0,1/2) \ 0,1/2,z \\
(4) & \ 4^+ (0,0,1/2) \ 1/2,0,z \\
(4) & \ 4^- (0,0,1/2) \ 1/2,0,z \\
(4) & \ 4^- (0,0,1/2) \ 1/2,0,z \\
(5) & \ 2 (0,1/2,0) \ 1/4,y,0 \\
(2) & \ 2 (1/2,1/2,0) \ x,1/4,0 \\
(2) & \ 2 (1/2,1/2,0) \ x,1/4,0 \\
(6) & \ 2 (1/2,1/2,0) \ x,1/4,0 \\
(7) & \ 2 (1/2,1/2,0) \ x,x,0 \\
(2) & \ 2 (1/2,1/2,0) \ x,x,0 \\
(8) & \ 2 \ x,x+1/2,0 \\
(2) & \ 2 \ x,x+1/2,0 \\
(9) & \ \bar{T} 1/4,1/4,1/4 \\
(T) & \ \bar{T} 1/2,1/2,1/2 \\
(10) & \ n (1/2,1/2,0) \ x,y,0 \\
(11) & \ 4^- 1/2,0,1/4 ; 1/2,0,1/4 \\
(4) & \ 4^- z 1/2,1/2,1/2 \\
(12) & \ 4^- 0,1/2,z ; 0,1/2,1/4 \\
(4) & \ 4^- z 1/2,1/2,1/2 \\
(13) & \ a (1/2,0,0) \ x,1/4,z \\
(m) & \ a (1/2,0,0) \ x,1/4,z \\
(14) & \ b (0,1/2,0) \ 1/4,y,0 \\
(15) & \ m \ x+1/2,x,z \\
(16) & \ g (1/2,1/2,0) \ x,x,z \\
(17) & \ m (1/2,1/2,0) \ x,x,z \\
\end{align*}
\]

For \((0,0,0)' +\) set

\[
\begin{align*}
(1) & \ t' (1/2,1/2,1/2) \\
(1) & \ t' (1/2,1/2,1/2) \\
(2) & \ 2' (0,0,0)' \ 1/4,1/4,z \\
(2) & \ 2' (0,0,0)' \ 1/4,1/4,z \\
(3) & \ 4^+ (0,0,0)' \ 0,1/2,z \\
(4) & \ 4^+ (0,0,0)' \ 1/2,0,z \\
(4) & \ 4^+ (0,0,0)' \ 1/2,0,z \\
(5) & \ 2' (0,1/2,0) \ 1/4,y,0 \\
(2) & \ 2' (1/2,1/2,0) \ x,1/4,0 \\
(2) & \ 2' (1/2,1/2,0) \ x,1/4,0 \\
(6) & \ 2' (1/2,1/2,0) \ x,1/4,0 \\
(7) & \ 2' (1/2,1/2,0) \ x,x,0 \\
(2) & \ 2' (1/2,1/2,0) \ x,x,0 \\
(8) & \ 2' \ x,x+1/2,0 \\
(2) & \ 2' \ x,x+1/2,0 \\
(9) & \ \bar{T} 1/4,1/4,1/4 \\
(T) & \ \bar{T} 1/2,1/2,1/2 \\
(10) & \ n' (1/2,1/2,0) \ x,y,0 \\
(11) & \ 4^- 1/2,0,1/4 ; 1/2,0,1/4 \\
(4) & \ 4^- z 1/2,1/2,1/2 \\
(12) & \ 4^- 0,1/2,z ; 0,1/2,1/4 \\
(4) & \ 4^- z 1/2,1/2,1/2 \\
(13) & \ a' (1/2,0,0) \ x,1/4,z \\
(m) & \ a' (1/2,0,0) \ x,1/4,z \\
(14) & \ b' (0,1/2,0) \ 1/4,y,0 \\
(15) & \ m' \ x+1/2,x,z \\
(16) & \ g' (1/2,1/2,0) \ x,x,z \\
(17) & \ m (1/2,1/2,0) \ x,x,z \\
\end{align*}
\]

For \((1/2,1/2,1/2)' +\) set

\[
\begin{align*}
(1) & \ t' (1/2,1/2,1/2) \\
(1) & \ t' (1/2,1/2,1/2) \\
(2) & \ 2' (0,0,1/2) \ 1/4,1/4,z \\
(2) & \ 2' (0,0,1/2) \ 1/4,1/4,z \\
(3) & \ 4^+ (0,0,1/2) \ 0,1/2,z \\
(4) & \ 4^+ (0,0,1/2) \ 1/2,0,z \\
(4) & \ 4^+ (0,0,1/2) \ 1/2,0,z \\
(5) & \ 2' (0,1/2,0) \ 1/4,y,0 \\
(2) & \ 2' (1/2,1/2,0) \ x,1/4,0 \\
(2) & \ 2' (1/2,1/2,0) \ x,1/4,0 \\
(6) & \ 2' (1/2,1/2,0) \ x,1/4,0 \\
(7) & \ 2' (1/2,1/2,0) \ x,x,0 \\
(2) & \ 2' (1/2,1/2,0) \ x,x,0 \\
(8) & \ 2' \ x,x+1/2,0 \\
(2) & \ 2' \ x,x+1/2,0 \\
(9) & \ \bar{T} 1/4,1/4,1/4 \\
(T) & \ \bar{T} 1/2,1/2,1/2 \\
(10) & \ n' (1/2,1/2,0) \ x,y,0 \\
(11) & \ 4^- 1/2,0,1/4 ; 1/2,0,1/4 \\
(4) & \ 4^- z 1/2,1/2,1/2 \\
(12) & \ 4^- 0,1/2,z ; 0,1/2,1/4 \\
(4) & \ 4^- z 1/2,1/2,1/2 \\
(13) & \ a' (1/2,0,0) \ x,1/4,z \\
(m) & \ a' (1/2,0,0) \ x,1/4,z \\
(14) & \ b' (0,1/2,0) \ 1/4,y,0 \\
(15) & \ m' \ x+1/2,x,z \\
(16) & \ g' (1/2,1/2,0) \ x,x,z \\
(17) & \ m (1/2,1/2,0) \ x,x,z \\
\end{align*}
\]

Generators selected

\((1); \ t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ t(1/2,1/2,1/2); (2); (3); (5); (9); 1'\)

Positions

\[
\begin{align*}
\text{Multiplicity,} & \quad \text{Wyckoff letter,} \\
\text{Site Symmetry.} & \quad \text{Coordinates}
\end{align*}
\]

\[
\begin{align*}
(0,0,0) + & \quad (1/2,1/2,1/2) + \\
(0,0,0)' + & \quad (1/2,1/2,1/2)' +
\end{align*}
\]
32  m  11'  (1) x,y,z [0,0,0]  (2) x̅,y̅,z [0,0,0]  (3) y,x,z [0,0,0]  (4) y̅,x̅,z [0,0,0]
   (5) x̅,y̅,z+1/2 [0,0,0]  (6) x̅,y̅,z+1/2 [0,0,0]  (7) y,x̅,z+1/2 [0,0,0]  (8) y̅,x̅,z+1/2 [0,0,0]
   (9) x̅,y̅,z [0,0,0]  (10) x,y,z [0,0,0]  (11) y,x̅,z [0,0,0]  (12) y̅,x̅,z [0,0,0]
   (13) x̅,y̅,z+1/2 [0,0,0]  (14) x̅,y̅,z+1/2 [0,0,0]  (15) y,x̅,z+1/2 [0,0,0]  (16) y,x,0,0,0)

16  l  ..m1'  x,x+1/2,z [0,0,0]  x̅,x+1/2,z [0,0,0]  x̅+1/2,x,z [0,0,0]  x̅+1/2,x̅,z [0,0,0]
   x̅,x+1/2,z+1/2 [0,0,0]  x,x+1/2,z+1/2 [0,0,0]  x+1/2,x,z+1/2 [0,0,0]  x+1/2,x̅,z+1/2 [0,0,0]

16  k  m..1'  x,y,0 [0,0,0]  x̅,y,0 [0,0,0]  y,x̅,0 [0,0,0]  y̅,x̅,0 [0,0,0]
   x̅,y,1/2 [0,0,0]  x,y,1/2 [0,0,0]  y,x,1/2 [0,0,0]  y̅,x̅,1/2 [0,0,0]

16  j  ..2.1'  x,0,1/4 [0,0,0]  x̅,0,1/4 [0,0,0]  0,x,1/4 [0,0,0]  0,x,1/4 [0,0,0]
   x̅,0,3/4 [0,0,0]  x,0,3/4 [0,0,0]  0,x̅,3/4 [0,0,0]  0,x,3/4 [0,0,0]

16  i  ..21'  x,x,1/4 [0,0,0]  x̅,x,1/4 [0,0,0]  x̅,x,1/4 [0,0,0]  x,x,1/4 [0,0,0]
   x̅,x̅,3/4 [0,0,0]  x,x̅,3/4 [0,0,0]  x,x̅,3/4 [0,0,0]  x,x,3/4 [0,0,0]

8   h  m.2m1'  x,x+1/2,0 [0,0,0]  x̅,x+1/2,0 [0,0,0]  x+1/2,x̅,0 [0,0,0]  x+1/2,x,0 [0,0,0]

8   g  2.mm1'  0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  0,1/2,z̅+1/2 [0,0,0]  1/2,0,z̅+1/2 [0,0,0]

8   f  4..1'  0,0,z [0,0,0]  0,0,z+1/2 [0,0,0]  0,0,z [0,0,0]  0,0,z+1/2 [0,0,0]

8   e  ..2/m1'  1/4,1/4,1/4 [0,0,0]  3/4,3/4,1/4 [0,0,0]  3/4,1/4,1/4 [0,0,0]  1/4,3/4,1/4 [0,0,0]

4   d  m.mm1'  0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]

4   c  4/m..1'  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]

4   b  42m1'  0,1/2,1/4 [0,0,0]  1/2,0,1/4 [0,0,0]

4   a  4221'  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4mm1'  a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,0,0]  p2mm1'  a* = b/2  b* = c/2
Origin at x,0,0

Along [1,1,0]  p2mm1'  a* = -(a + b)/2  b* = c/2
Origin at x,x,0

140.2.1197 - 3 - 2543
I4/m'cm
140.3.1198

4/m'nm
I4/m'2'/c2'/m

Tetragonal

Origin at center (4/m') at 4/m'c2'/c

Asymmetric unit
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y < 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(5) 2’ 0,y,1/4
(2z | 0,0,1/2)’

(9) 1’ 0,0,0
(1 | 0,0,0)’

(13) c (0,0,1/2) x,0,z
(mz | 0,0,1/2)

(2) 2 0,0,z
(2z | 0,0,0)

(6) 2’ x,0,1/4
(2z | 0,0,1/2)’

(10) m’ x,y,0
(mz | 0,0,0)’

(14) c (0,0,1/2) 0,y,z
(mz | 0,0,1/2)

(3) 4’ 0,0,z
(4z | 0,0,0)

(7) 2’ x,x,1/4
(2xy | 0,0,1/2)’

(11) 4’ 0,0,z; 0,0,0
(4z | 0,0,0)’

(12) 4’ 0,0,0; 0,0,0
(4z | 0,0,0)’

(4) 4’ 0,0,z
(4z | 0,0,0)

(8) 2’ x,x,1/4
(2xy | 0,0,1/2)’

(15) c (0,0,1/2) x,x,z
(mxy | 0,0,1/2)

(16) c (0,0,1/2) x,x,z
(mxy | 0,0,1/2)
Continued

For (1/2,1/2,1/2) + set

<table>
<thead>
<tr>
<th>Positions selected</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (1/2,1/2,1/2)</td>
<td>(0,0,0) + (1/2,1/2,1/2)</td>
</tr>
<tr>
<td>(2) 2' 0,0,1/2</td>
<td>1/4,1/4,z</td>
</tr>
<tr>
<td>(3) 4' 0,0,1/2</td>
<td>0,1/2,z</td>
</tr>
<tr>
<td>(4) 4' 0,0,1/2</td>
<td>1/2,0,z</td>
</tr>
<tr>
<td>(5) 2' 0,1/2,0</td>
<td>1/4,y,0</td>
</tr>
<tr>
<td>(6) 2' 1/2,0,0</td>
<td>x,1/4,0</td>
</tr>
<tr>
<td>(7) 2' 1/2,1/2,0</td>
<td>x,0,0</td>
</tr>
<tr>
<td>(8) 2' x,x+1/2,0</td>
<td></td>
</tr>
<tr>
<td>(9) 1/4,1/4,1/4</td>
<td>(10) n' 1/2,1/2,0</td>
</tr>
<tr>
<td>(11) 4' 1/2,0,0, z</td>
<td>1/2,0,1/4</td>
</tr>
<tr>
<td>(12) 4' 0,1/2,0, z</td>
<td>0,1/2,1/2</td>
</tr>
<tr>
<td>(13) a 1/2,0,0</td>
<td>x,1/4,z</td>
</tr>
<tr>
<td>(14) b 0,1/2,0</td>
<td>1/4,y,z</td>
</tr>
<tr>
<td>(15) m</td>
<td>x+1/2,x,z</td>
</tr>
<tr>
<td>(16) g 1/2,1/2,0</td>
<td>x,x,z</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Multiplicities:

<table>
<thead>
<tr>
<th>Generators</th>
<th>Multiplicity</th>
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</thead>
<tbody>
<tr>
<td>m 1</td>
<td>32</td>
</tr>
<tr>
<td>m'..</td>
<td>16</td>
</tr>
<tr>
<td>h m'..2'm</td>
<td>8</td>
</tr>
<tr>
<td>g 2.mm</td>
<td>8</td>
</tr>
<tr>
<td>f 4..</td>
<td>8</td>
</tr>
<tr>
<td>e ..2'm</td>
<td>8</td>
</tr>
<tr>
<td>d m.mm</td>
<td>4</td>
</tr>
</tbody>
</table>

Wyckoff letter, Site Symmetry, Coordinates.
4 c 4/m'.. 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]
4 b 4'2'm 0,1/2,1/4 [0,0,0] 1/2,0,1/4 [0,0,0]
4 a 42'2' 0,0,1/4 [0,0,w] 0,0,3/4 [0,0,w]

Symmetry of Special Projections

Along [0,0,1]  p4mm1'   Along [1,0,0]  p2m..   Along [1,1,0]  p2mm1'
\( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  \( a^* = (-a + b)/2 \)  \( b^* = c/2 \)
Origin at 0,0,z Origin at 1/4,1/4 Origin at x,x,0
**Origin** at center (4/m) at 4/mc'2/c

**Asymmetric unit**
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ 1/2 - x

**Symmetry Operations**

For (0,0,0) + set

1. 1
   (1 | 0,0,0)

2. 2  0,0,z
   (2z | 0,0,0)

3. 4'  0,0,z
   (4z | 0,0,0)

4. 4  0,0,z
   (4z | 0,0,0)

5. 2'  0,y,1/4
   (2' | 0,0,1/2)

6. 2'  x,0,1/4
   (2' | 0,0,1/2)

7. 2  x,y,1/4
   (2 | 0,0,1/2)

8. 2  x,y,1/4
   (2 | 0,0,1/2)

9. 1  0,0,0
   (1 | 0,0,0)

10. m  x,y,0
    (mz | 0,0,0)

11. 4'  0,0,z; 0,0,0
    (4z | 0,0,0)

12. 4'  0,0,z; 0,0,0
    (4z | 0,0,0)

13. c' (0,0,1/2)  x,0,z
    (m | 0,0,1/2)

14. c' (0,0,1/2)  0,y,z
    (m | 0,0,1/2)

15. c (0,0,1/2)  x,0,z
    (mxy | 0,0,1/2)

16. c (0,0,1/2)  x,0,z
    (mxy | 0,0,1/2)
For \((1/2,1/2,1/2) + \) set

\[
\begin{align*}
(1) \ t (1/2,1/2,1/2) & (2) \ 2 (0,0,1/2) 1/4,1/4,z \\
(1/2,1/2,1/2) & (2) \ 1/2,1/2,1/2) \\
(1) \ t (1/2,1/2,1/2) & (3) \ 4^+ \ (0,0,1/2) 0,1/2,z \\
(2) \ 1/2,1/2,1/2) & (4) \ 4^+ \ (0,0,1/2) 1/2,0,z \\
(2) \ 1/2,1/2,1/2) & (4) \ 1/2,1/2,1/2) \\
(5) \ 2^* (0,1/2,0) 1/4,y,0 & (6) \ 2^* (1/2,0,0) x,1/4,0 \\
(2) \ 1/2,1/2,0) & (7) \ 2 (1/2,1/2,0) x,x,0 \\
(2) \ 1/2,1/2,0) & (8) \ 2 x,x+1/2,0 \\
(2) \ 1/2,1/2,0) & (2) \ 1/2,1/2,0) \\
(9) \ 1/4,1/4,1/4 & (10) \ 1/4,1/4,1/4 \\
(1/2,1/2,1/2) & (11) \ 1/2,0,1/4 \\
(1/2,1/2,1/2) & (12) \ 1/2,0,1/4 \\
(4) \ 1/2,1/2,1/2) & (4) \ 1/2,1/2,1/2) \\
(4) \ 1/2,1/2,1/2) & (4) \ 1/2,1/2,1/2) \\
(13) \ a^* (1/2,0,0) x,1/4,z & (14) \ b^* (0,1/2,0) 1/4,y,z \\
(m) \ 1/2,1/2,0) & (15) \ m x+1/2,x,z \\
(m) \ 1/2,1/2,0) & (16) \ g (1/2,1/2,0) x,x,z \\
(m) \ 1/2,1/2,0) & (m) \ 1/2,1/2,0) \\
\end{align*}
\]

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z+1/2 [u,v,w]</td>
<td>(6) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,y,z [u,v,w]</td>
<td>(10) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(13) x,y,z+1/2 [u,v,w]</td>
<td>(14) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>16 l ..m</td>
<td>x,x+1/2,z [u,u,0]</td>
<td>x,x+1/2,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x+1/2,z [u,u,0]</td>
<td>x+1/2,x,z [u,u,0]</td>
</tr>
<tr>
<td>16 k m..</td>
<td>x,y,0 [0,0,w]</td>
<td>x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,y,1/2 [0,0,w]</td>
<td>y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>16 j ..2'</td>
<td>x,0,1/4 [0,v,w]</td>
<td>x,0,1/4 [0,v,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [0,v,w]</td>
<td>x,0,3/4 [0,v,w]</td>
</tr>
<tr>
<td>16 i ..2</td>
<td>x,x,1/4 [u,u,0]</td>
<td>x,x,1/4 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,3/4 [u,u,0]</td>
<td>x,x,3/4 [u,u,0]</td>
</tr>
<tr>
<td>8 h m.2m</td>
<td>x,x,1/2,0 [0,0,0]</td>
<td>x,x,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,x+1/2,0 [0,0,0]</td>
<td>x+1/2,x,0 [0,0,0]</td>
</tr>
<tr>
<td>8 g 2.mm</td>
<td>0,1/2,z [0,0,0]</td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>8 f ..4'</td>
<td>0,0,3 [0,0,0]</td>
<td>0,0,3 [0,0,0]</td>
</tr>
<tr>
<td>8 e ..2/m</td>
<td>1/4,1/4,1/4 [u,u,0]</td>
<td>3/4,3/4,1/4 [u,u,0]</td>
</tr>
<tr>
<td>4 d m.mm</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along $[0,0,1]$ $p4'm'm'$

$\mathbf{a}^* = \frac{\mathbf{a} - \mathbf{b}}{2}$  
$\mathbf{b}^* = \frac{\mathbf{a} + \mathbf{b}}{2}$

Origin at 0,0,z

Along $[1,0,0]$ $p2m'm'$

$\mathbf{a}^* = \frac{\mathbf{b}}{2}$  
$\mathbf{b}^* = \frac{\mathbf{c}}{2}$

Origin at x,0,0

Along $[1,1,0]$ $p2mm'1'$

$\mathbf{a}^* = \frac{-\mathbf{a} + \mathbf{b}}{2}$  
$\mathbf{b}^* = \frac{\mathbf{c}}{2}$

Origin at x,x,0
I4'/mcm'  
140.5.1200

I4'/mmm'  
4'/m2/c2'/m'

Tetragonal

Origin at center (4'/m ) at 4'/mc21'/c'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

1. 1  (1) 1 0,0,0
2. 2  0,0,z  (2) 2 0,0,0  (2z 0,0,0)
3. 4'  0,0,z  (3) 4 0,0,0'  (4 0,0,0')
4. 4'  0,0,z  (4 0,0,0')  (4 0,0,0)
5. 2  0,y,1/4  (5) 2 0,0,1/2  (2z 0,0,1/2)
6. 2'  x,0,1/4  (6) 2 0,0,1/2  (2z 0,0,1/2)
7. 2'  x,x,1/4  (7) 2' 0,0,1/2  (2z 0,0,1/2)
8. 2'  x,x,1/4  (8) 2' 0,0,1/2  (2z 0,0,1/2)
9. 0,0,0  (9) 0,0,0  (1 0,0,0)
10. m  x,y,0  (10) m 0,0,0  (mz 0,0,0)
11. 4'  0,0,z; 0,0,0  (11) 4' 0,0,0'  (4'z 0,0,0')
12. 4'  0,0,z; 0,0,0  (12) 4' 0,0,0'  (4'z 0,0,0')
13. c (0,0,1/2)  x,0,z  (m 0,0,1/2)
14. c (0,0,1/2)  0,y,z  (m 0,0,1/2)
15. c' (0,0,1/2)  x,x,z  (m 0,0,1/2)
16. c' (0,0,1/2)  x,x,z  (m 0,0,1/2)
Continued

For \((1/2,1/2,1/2) + \text{ set}\)

<table>
<thead>
<tr>
<th>Positions selected</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1; t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9)).</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Generators</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) (x, \bar{y}, \bar{z}, [u, v, w])</td>
<td>32 (m) (1)</td>
</tr>
<tr>
<td>(2) (\bar{x}, \bar{y}, \bar{z}, [\bar{u}, \bar{v}, \bar{w}])</td>
<td>(1, x, y, z, [u, v, w])</td>
</tr>
<tr>
<td>(3) (\bar{y}, x, z, [v, u, w])</td>
<td>(1/2,1/2,1/2, z)</td>
</tr>
<tr>
<td>(4) (\bar{y}, \bar{x}, \bar{z}, [v, u, w])</td>
<td>(0, 0, 0, z+1/2)</td>
</tr>
<tr>
<td>(5) (x, \bar{y}, z+1/2, [u, v, w])</td>
<td>(x, y, 0, [0, 0, w])</td>
</tr>
<tr>
<td>(6) (x, \bar{y}, z+1/2, [u, v, w])</td>
<td>(x, y, 1/2, [0, 0, w])</td>
</tr>
<tr>
<td>(7) (x, y, x, 1/2, [0, 0, w])</td>
<td>(y, x, z, [v, u, w])</td>
</tr>
<tr>
<td>(8) (x, y, x, 1/2, [0, 0, w])</td>
<td>(y, x, 1/2, [0, 0, w])</td>
</tr>
<tr>
<td>(9) (x, y, z, [u, v, w])</td>
<td>(x, 0, 1/4, [u, 0, 0])</td>
</tr>
<tr>
<td>(10) (x, y, z, [u, v, w])</td>
<td>(x, 0, 3/4, [u, 0, 0])</td>
</tr>
<tr>
<td>(11) (x, y, x, 1/4, [u, 0, 0])</td>
<td>(x, 3/4, [u, 0, 0])</td>
</tr>
<tr>
<td>(12) (x, y, z, [v, u, w])</td>
<td>(x, x, 1/4, [u, u, w])</td>
</tr>
<tr>
<td>(13) (x, y, z+1/2, [v, u, w])</td>
<td>(x, x, 1/4, [u, u, w])</td>
</tr>
<tr>
<td>(14) (x, y, z+1/2, [v, u, w])</td>
<td>(x, x, 3/4, [u, u, w])</td>
</tr>
<tr>
<td>(15) (x, y, x, 1/2, [v, u, w])</td>
<td>(x, x, 3/4, [u, u, w])</td>
</tr>
<tr>
<td>(16) (x, y, z, [v, u, w])</td>
<td>(x, x, 1/4, [u, u, w])</td>
</tr>
<tr>
<td>(17) (x, y, x, 1/2, [v, u, w])</td>
<td>(x, x, 3/4, [u, u, w])</td>
</tr>
<tr>
<td>(18) (x, y, x, 1/2, [v, u, w])</td>
<td>(x, x, 3/4, [u, u, w])</td>
</tr>
<tr>
<td>(19) (x, y, x, 1/2, [v, u, w])</td>
<td>(x, x, 3/4, [u, u, w])</td>
</tr>
<tr>
<td>(20) (x, y, x, 1/2, [v, u, w])</td>
<td>(x, x, 3/4, [u, u, w])</td>
</tr>
</tbody>
</table>

\[140.5.1200 - 2 - 2551\]
Continued

140.5.1200

\[ \text{l4}'/\text{mcm}' \]

4 \hspace{0.5cm} c \hspace{0.5cm} \text{4'/m}.. \hspace{0.5cm} 0,0,0 [0,0,0] \hspace{0.5cm} 0,0,1/2 [0,0,0]

4 \hspace{0.5cm} b \hspace{0.5cm} \overline{4}'2m' \hspace{0.5cm} 0,1/2,1/4 [0,0,0] \hspace{0.5cm} 1/2,0,1/4 [0,0,0]

4 \hspace{0.5cm} a \hspace{0.5cm} \text{4'22'} \hspace{0.5cm} 0,0,1/4 [0,0,0] \hspace{0.5cm} 0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] \( \text{p4mm}' \)
\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]
Origin at 0,0,z

Along [1,0,0] \( \text{p}_{c*2mm} \)
\[ \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x,1/4,0

Along [1,1,0] \( \text{p2'2m}' \)
\[ \mathbf{a}^* = -\mathbf{c}/2 \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]
Origin at x,x,0
**Origin** at center (4'/m') at 4'/m'c'2'/c

**Asymmetric unit**

\[ \begin{align*}
0 & \leq x \leq 1/2; \\
0 & \leq y \leq 1/2; \\
0 & \leq z \leq 1/4; \\
y & \leq 1/2 - x
\end{align*} \]

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1,0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2_z,0,0,0) \\
(3) & \quad 4^{+} \quad 0,0,z \\
& \quad (4_z,0,0,0)' \\
(4) & \quad 4^{-} \quad 0,0,z \\
& \quad (4_z^{-1},0,0,0)'
\end{align*}
\]

\[
\begin{align*}
(5) & \quad 2 \quad 0,y,1/4 \\
& \quad (2_y,0,0,1/2) \\
(6) & \quad 2 \quad x,0,1/4 \\
& \quad (2_x,0,0,1/2) \\
(7) & \quad 2' \quad x,x,1/4 \\
& \quad (2_{xy},0,0,1/2)'
\end{align*}
\]

\[
\begin{align*}
(8) & \quad 2' \quad x,x,1/4 \\
& \quad (2_{xy},0,0,1/2)'
\end{align*}
\]

\[
\begin{align*}
(9) & \quad \bar{1} \quad 0,0,0 \\
& \quad (1,0,0,0)'
\end{align*}
\]

\[
\begin{align*}
(10) & \quad m' \quad x,y,0 \\
& \quad (m_x,0,0,0)'
\end{align*}
\]

\[
\begin{align*}
(11) & \quad \bar{4} \quad 0,0,z; 0,0,0 \\
& \quad (4_z,0,0,0)
\end{align*}
\]

\[
\begin{align*}
(12) & \quad \bar{4} \quad 0,0,z; 0,0,0 \\
& \quad (4_z^{-1},0,0,0)
\end{align*}
\]

\[
\begin{align*}
(13) & \quad c' \quad (0,0,1/2) \quad x,0,z \\
& \quad (m_y,0,0,1/2)'
\end{align*}
\]

\[
\begin{align*}
(14) & \quad c' \quad (0,0,1/2) \quad 0,y,z \\
& \quad (m_y,0,0,1/2)'
\end{align*}
\]

\[
\begin{align*}
(15) & \quad c \quad (0,0,1/2) \quad x,x,z \\
& \quad (m_x,0,0,1/2)
\end{align*}
\]

\[
\begin{align*}
(16) & \quad c \quad (0,0,1/2) \quad x,x,z \\
& \quad (m_x,0,0,1/2)
\end{align*}
\]
For \((1/2,1/2,1/2)+\) set

\[
\begin{align*}
(1) & \ t(1/2,1/2,1/2) \\
(2) & \ 2 (0,0,1/2) \hspace{1cm} 1/4,1/4,z \\
(3) & \ 4^+ \ (0,0,1/2) \hspace{1cm} 0,1/2,z \\
(4) & \ 4^+ \ (0,0,1/2) \hspace{1cm} 1/2,0,z \\
(5) & \ 2 (0,1/2,0) \hspace{1cm} 1/4,y,0 \\
(6) & \ 2 (1/2,0,0) \hspace{1cm} x,1/4,0 \\
(7) & \ 2' (1/2,1/2,0) \hspace{1cm} x,x,0 \\
(8) & \ 2' \ x,x+1/2,0 \\
(9) & \ \bar{T} \hspace{1cm} \bar{1}/4,1/4,1/4 \\
(10) & \ n' (1/2,1/2,0) \hspace{1cm} x,y,1/4 \\
(11) & \ \bar{4}^+ \ 1/2,0,z; \hspace{1cm} 1/2,0,1/4 \\
(12) & \ \bar{4} \hspace{1cm} 0,1/2,z; \hspace{1cm} 0,1/2,1/4 \\
(13) & \ a' (1/2,0,0) \hspace{1cm} x,1/4,z \\
(14) & \ b' (0,1/2,0) \hspace{1cm} 1/4,y,z \\
(15) & \ m \hspace{1cm} x+1/2,x,z \\
(16) & \ g (1/2,1/2,0) \hspace{1cm} x,x,z
\end{align*}
\]

Generators selected \((1); \ t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ t(1/2,1/2,1/2); (2); (3); (5); (9).\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(32)</td>
<td>(m \ 1) (x,y,z [u,v,w])</td>
<td>((0,0,0) + (1/2,1/2,1/2) + )</td>
</tr>
<tr>
<td>(16)</td>
<td>(l \ ..m) (x,x+1/2,z [u,u,0])</td>
<td>(x,x+1/2,z [u,u,0])</td>
</tr>
</tbody>
</table>

### Generators selected

\((1); \ t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ t(1/2,1/2,1/2); (2); (3); (5); (9).\)
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>442m</th>
<th>442m'</th>
<th>22m</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0,0,0</td>
<td>0,0,1/4</td>
<td>0,1/2,1/4</td>
</tr>
<tr>
<td>b</td>
<td>0,0,1/4</td>
<td>0,0,3/4</td>
<td></td>
</tr>
</tbody>
</table>

#### Along [0,0,1] p4mm'
- \( a^* = (a - b)/2 \)
- \( b^* = (a + b)/2 \)

#### Along [1,0,0] p2m'm'
- \( a^* = b/2 \)
- \( b^* = c/2 \)

#### Along [1,1,0] p2mm1'
- \( a^* = (-a + b)/2 \)
- \( b^* = c/2 \)
I4/mc' \, m'  
140.7.1202  

4/mm' \, m'  
I4/m2'/c'2'/m'  

**Origin** at center (4/m) at 4/mc'2'/c'

**Asymmetric unit**  
0 \leq x \leq 1/2;  
0 \leq y \leq 1/2;  
0 \leq z \leq 1/4;  
y \leq 1/2 - x

**Symmetry Operations**

For (0,0,0) + set

1. \( (1) \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \)
2. \( (2) \begin{pmatrix} 2 & 0,0,z \\ z & 0,0,0 \end{pmatrix} \)
3. \( (3) \begin{pmatrix} 4^+ & 0,0,z \\ 4_z & 0,0,0 \end{pmatrix} \)
4. \( (4) \begin{pmatrix} 4^- & 0,0,z \\ 4_z^{-1} & 0,0,0 \end{pmatrix} \)
5. \( (5) 2^\prime \begin{pmatrix} 0,0,1/4 \\ 0,0,1/2 \end{pmatrix} \)
6. \( (6) 2^\prime \begin{pmatrix} x,0,1/4 \\ z,0,0,1/2 \end{pmatrix} \)
7. \( (7) 2^\prime \begin{pmatrix} x,x,1/4 \\ 2_{xy} & 0,0,1/2 \end{pmatrix} \)
8. \( (8) 2^\prime \begin{pmatrix} x,x,1/4 \\ 2_{xy} & 0,0,1/2 \end{pmatrix} \)
9. \( (9) \begin{pmatrix} 1 & 0,0,0 \end{pmatrix} \)
10. \( (10) \begin{pmatrix} m & x,y,0 \\ m_z & 0,0,0 \end{pmatrix} \)
11. \( (11) \begin{pmatrix} 4^+ & 0,0,z; 0,0,0 \\ 4_z & 0,0,0 \end{pmatrix} \)
12. \( (12) \begin{pmatrix} 4^- & 0,0,z; 0,0,0 \\ 4_z^{-1} & 0,0,0 \end{pmatrix} \)
13. \( (13) \begin{pmatrix} c' & (0,0,1/2) \begin{pmatrix} x,0,z \\ m_y & 0,0,1/2 \end{pmatrix} \)
14. \( (14) \begin{pmatrix} c' & (0,0,1/2) \begin{pmatrix} 0,y,z \\ m_y & 0,0,1/2 \end{pmatrix} \)
15. \( (15) \begin{pmatrix} c' & (0,0,1/2) \begin{pmatrix} x,x,z \\ m_{xy} & 0,0,1/2 \end{pmatrix} \)
16. \( (16) \begin{pmatrix} c' & (0,0,1/2) \begin{pmatrix} x,x,z \\ m_{xy} & 0,0,1/2 \end{pmatrix} \)

Tetragonal
Continued

For $(1/2,1/2,1/2) + set$

<table>
<thead>
<tr>
<th>(1) t (1/2,1/2,1/2)</th>
<th>(2) 2 (0,0,1/2)</th>
<th>1/4,1/4,z</th>
<th>(3) $4^*$ (0,0,1/2)</th>
<th>0,1/2,z</th>
<th>(4) $4^*$ (0,0,1/2)</th>
<th>1/2,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1/2,1/2,1/2)$</td>
<td>$(2_z,1/2,1/2,1/2)$</td>
<td></td>
<td>$(4_z,1/2,1/2,1/2)$</td>
<td></td>
<td>$(4_z,1/2,1/2,1/2)$</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(5) $2'$ (0,1/2,0)</th>
<th>1/4,y,0</th>
<th>(2) $2'$ (1/2,0,0)</th>
<th>x,1/4,0</th>
<th>(7) $2'$ (1/2,1/2,0)</th>
<th>x,x,0</th>
<th>(8) $2'$ x,x+1/2,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(2_z,1/2,1/2,0)''$</td>
<td></td>
<td>$(2_z,1/2,1/2,0)''$</td>
<td></td>
<td>$(2_{xy},1/2,1/2,0)''$</td>
<td></td>
<td>$(2_{xy},1/2,1/2,0)''$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(9) $\bar{T}$ 1/4,1/4,1/4</th>
<th>(10) n (1/2,1/2,0)</th>
<th>x,y,1/4</th>
<th>(11) $\bar{4}^*$ 1/2,0,1/4</th>
<th>1/2,0,1/4</th>
<th>(12) $\bar{4}^*$ 0,1/2,1/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(2 \bar{z},1/2,1/2,1/2)$</td>
<td>$(m_{xy},1/2,1/2,1/2)$</td>
<td></td>
<td>$(4_z,1/2,1/2,1/2)$</td>
<td></td>
<td>$(4_z,1/2,1/2,1/2)$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(13) a' (1/2,0,0)</th>
<th>x,1/4,z</th>
<th>(14) b' (0,1/2,0)</th>
<th>1/4,y,z</th>
<th>(15) m' x+1/2,x,z</th>
<th>(16) g' (1/2,1/2,0)</th>
<th>x,x,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(m_{xy},1/2,1/2,0)''$</td>
<td></td>
<td>$(m_{xy},1/2,1/2,0)''$</td>
<td></td>
<td>$(m_{xy},1/2,1/2,0)''$</td>
<td></td>
<td>$(m_{xy},1/2,1/2,0)''$</td>
</tr>
</tbody>
</table>

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 m 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) $\bar{x},\bar{y},\bar{z}$ [u,v,w]</td>
<td>(3) $\bar{y},\bar{x},\bar{z}$ [v,u,w]</td>
</tr>
<tr>
<td>(5) $\bar{x},\bar{y},\bar{z}+1/2$ [u,v,w]</td>
<td>(6) $\bar{x},\bar{y},\bar{z}+1/2$ [u,v,w]</td>
<td>(7) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]</td>
</tr>
<tr>
<td>(9) $\bar{x},\bar{y},\bar{z}$ [u,v,w]</td>
<td>(10) $\bar{x},\bar{y},\bar{z}$ [u,v,w]</td>
<td>(11) $\bar{y},\bar{x},\bar{z}$ [v,u,w]</td>
</tr>
<tr>
<td>(13) $\bar{x},\bar{y},\bar{z}+1/2$ [u,v,w]</td>
<td>(14) $\bar{x},\bar{y},\bar{z}+1/2$ [u,v,w]</td>
<td>(15) $\bar{y},\bar{x},\bar{z}+1/2$ [v,u,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>16 l .m'</th>
<th>$x,x+1/2,z,[u,u,w]$</th>
<th>$\bar{x},\bar{x}+1/2,z,[u,u,w]$</th>
<th>$x+1/2,x,z,[u,u,w]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16 k .m..</td>
<td>$x,y,0,[0,0,w]$</td>
<td>$\bar{x},\bar{y},0,[0,0,w]$</td>
<td>$\bar{y},\bar{x},0,[0,0,w]$</td>
</tr>
<tr>
<td>16 j .2'</td>
<td>$x,0,1/4,[0,v,w]$</td>
<td>$\bar{x},0,1/4,[0,v,w]$</td>
<td>$0,x,1/4,[v,0,w]$</td>
</tr>
<tr>
<td>16 i .2'</td>
<td>$x,x,1/4,[u,u,w]$</td>
<td>$\bar{x},\bar{x},1/4,[u,u,w]$</td>
<td>$\bar{x},x,1/4,[u,u,w]$</td>
</tr>
<tr>
<td>8 h m.2'm'</td>
<td>$x,x+1/2,0,[0,0,w]$</td>
<td>$\bar{x},\bar{x}+1/2,0,[0,0,w]$</td>
<td>$x+1/2,\bar{x},0,[0,0,w]$</td>
</tr>
<tr>
<td>8 g 2.m'm'</td>
<td>0,1/2,z,[0,0,w]</td>
<td>1/2,0,z,[0,0,w]</td>
<td>0,1/2,\bar{z}+1/2,[0,0,w]</td>
</tr>
<tr>
<td>8 f 4.m..'</td>
<td>0,0,z,[0,0,w]</td>
<td>0,0,\bar{z}+1/2,[0,0,w]</td>
<td>0,0,z,[0,0,w]</td>
</tr>
<tr>
<td>8 e .2'm'</td>
<td>1/4,1/4,1/4,[u,u,w]</td>
<td>3/4,3/4,1/4,[u,u,w]</td>
<td>3/4,1/4,1/4,[u,u,w]</td>
</tr>
<tr>
<td>4 d m.m'm'</td>
<td>0,1/2,0,[0,0,w]</td>
<td>1/2,0,0,[0,0,w]</td>
<td></td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along ([0,0,1])</td>
<td>(p4mm')</td>
<td>(0,0,z)</td>
</tr>
<tr>
<td>(a^* = (a - b)/2)</td>
<td>(b^* = (a + b)/2)</td>
<td></td>
</tr>
<tr>
<td>Along ([1,0,0])</td>
<td>(p2'mm')</td>
<td>(x,0,0)</td>
</tr>
<tr>
<td>(a^* = -c/2)</td>
<td>(b^* = b/2)</td>
<td></td>
</tr>
<tr>
<td>Along ([1,1,0])</td>
<td>(p2'mm')</td>
<td>(x,x,0)</td>
</tr>
<tr>
<td>(a^* = -c/2)</td>
<td>(b^* = (-a + b)/2)</td>
<td></td>
</tr>
</tbody>
</table>

\(4\ c\ 4/m..\ 0,0,0\ [0,0,w]\ 0,0,1/2\ [0,0,w]\)

\(4\ b\ 42'm'\ 0,1/2,1/4\ [0,0,w]\ 1/2,0,1/4\ [0,0,w]\)

\(4\ a\ 42'2'\ 0,0,1/4\ [0,0,w]\ 0,0,3/4\ [0,0,w]\)
Origin at center (4/m') at 4'/m'c2'/c'

Asymmetric unit

\[ \begin{align*}
0 \leq x &\leq 1/2; \\
0 \leq y &\leq 1/2; \\
0 \leq z &\leq 1/4; \\
y &\leq 1/2 - x
\end{align*} \]

Symmetry Operations

For \((0,0,0) + \) set

\begin{align*}
(1) &
1 \\
& (1|0,0,0) \\
(5) &
2' \\
& 0,y,1/4 \\
& (2_{y'}|0,0,1/2)' \\
(9) &
\overline{3}' \\
& 0,0,0 \\
& (1|0,0,0)' \\
(13) &
c (0,0,1/2) \\
& x,0,z \\
& (m_{y'}|0,0,1/2) \\
(2) &
2 \\
& 0,0,z \\
& (2_{z}|0,0,0) \\
(6) &
2' \\
& x,0,1/4 \\
& (2_{x'}|0,0,1/2)' \\
(10) &
m' \\
& x,y,0 \\
& (m_{z}|0,0,0)' \\
(14) &
c (0,0,1/2) \\
& 0,y,z \\
& (m_{x}|0,0,1/2) \\
(3) &
4^{+} \\
& 0,0,z \\
& (4_{z}|0,0,0)' \\
(7) &
2 \\
& x,x,1/4 \\
& (2_{x'}|0,0,1/2) \\
(11) &
\overline{4}^{+} \\
& 0,0,z; 0,0,0 \\
& (4_{z}|0,0,0) \\
(15) &
c' (0,0,1/2) \\
& x,x,z \\
& (m_{y}|0,0,1/2)' \\
(4) &
4^{-} \\
& 0,0,z \\
& (4_{z}^{-}|0,0,0)' \\
(8) &
2 \\
& x,x,1/4 \\
& (2_{x'}|0,0,1/2) \\
(12) &
\overline{4}^{-} \\
& 0,0,z; 0,0,0 \\
& (4_{z}^{-}|0,0,0) \end{align*}
For $(1/2,1/2,1/2) + \text{set}$

(1) $t(1/2,1/2,1/2)$  
(2) $t(0,0,1/2)$  
(3) $4^+ (0,0,1/2)$  
(4) $4^+ (0,0,1/2)$  
(5) $2' (0,1/2,0)$  
(6) $2' (1/2,0,0)$  
(7) $2 (1/2,1/2,0)$  
(8) $2 (0,1/2,0)$  
(9) $\bar{1}$  
(10) $n' (1/2,1/2,0)$  
(11) $4\bar{m}' (1/2,1/2,0)$  
(12) $4\bar{m}' (0,1/2,0)$  
(13) $a (1/2,0,0)$  
(14) $b (0,1/2,0)$  
(15) $m' (1/2,1/2,0)$  
(16) $g' (1/2,1/2,0)$

**Generators selected**

$(1); t(1,0,0); t(0,1,0); t(1/2,1/2,1/2); (2); (3); (5); (9).$

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry, Coordinates

<table>
<thead>
<tr>
<th>m</th>
<th>1</th>
<th>(1) $x,y,z [u,v,w]$</th>
<th>(2) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$</th>
<th>(3) $\bar{y},x,z [v,u,w]$</th>
<th>(4) $y,x,z [\bar{v},\bar{u},\bar{w}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>m</td>
<td>(1) $x,y,z [u,v,w]$</td>
<td>(2) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$</td>
<td>(3) $\bar{y},x,z [v,u,w]$</td>
<td>(4) $y,x,z [\bar{v},\bar{u},\bar{w}]$</td>
</tr>
<tr>
<td>16</td>
<td>m'</td>
<td>$x+1/2,z [u,u,w]$</td>
<td>$\bar{x}+1/2,z [\bar{u},\bar{u},\bar{w}]$</td>
<td>$x+1/2,z [u,u,w]$</td>
<td>$\bar{x}+1/2,z [\bar{u},\bar{u},\bar{w}]$</td>
</tr>
<tr>
<td>16</td>
<td>m''</td>
<td>$x,y,0 [u,v,0]$</td>
<td>$\bar{x},\bar{y},\bar{0} [\bar{u},\bar{v},\bar{0}]$</td>
<td>$y,\bar{x},0 [v,\bar{u},0]$</td>
<td>$\bar{y},x,0 [\bar{v},u,0]$</td>
</tr>
<tr>
<td>16</td>
<td>m'''</td>
<td>$x,0,1/4 [0,v,w]$</td>
<td>$\bar{x},0,1/4 [\bar{0},\bar{v},\bar{w}]$</td>
<td>$0,x,1/4 [v,0,\bar{w}]$</td>
<td>$\bar{0},x,1/4 [\bar{v},0,\bar{w}]$</td>
</tr>
<tr>
<td>16</td>
<td>m''''</td>
<td>$\bar{x},x,1/4 [u,u,0]$</td>
<td>$x,\bar{x},1/4 [u,0,\bar{u}]$</td>
<td>$\bar{x},x,1/4 [u,u,0]$</td>
<td>$x,\bar{x},1/4 [u,0,\bar{u}]$</td>
</tr>
<tr>
<td>8</td>
<td>m'.2m'</td>
<td>$x+1/2,0 [u,u,0]$</td>
<td>$\bar{x}+1/2,0 [\bar{u},\bar{u},\bar{0}]$</td>
<td>$\bar{x}+1/2,0 [\bar{u},\bar{u},\bar{0}]$</td>
<td>$x+1/2,0 [u,u,0]$</td>
</tr>
<tr>
<td>8</td>
<td>m'.2m''</td>
<td>$0,1/2,z [0,0,\bar{w}]$</td>
<td>$1/2,0,z [0,0,\bar{w}]$</td>
<td>$0,1/2,z [0,0,\bar{w}]$</td>
<td>$1/2,0,z [0,0,\bar{w}]$</td>
</tr>
<tr>
<td>8</td>
<td>m'.2m'''</td>
<td>$0,0,z [0,0,\bar{0}]$</td>
<td>$0,0,z [0,0,\bar{0}]$</td>
<td>$0,0,z [0,0,\bar{0}]$</td>
<td>$0,0,z [0,0,\bar{0}]$</td>
</tr>
<tr>
<td>8</td>
<td>m'.2m''''</td>
<td>$1/4,1/4,1/4 [0,0,0]$</td>
<td>$3/4,3/4,1/4 [0,0,0]$</td>
<td>$3/4,3/4,1/4 [0,0,0]$</td>
<td>$1/4,3/4,1/4 [0,0,0]$</td>
</tr>
<tr>
<td>4</td>
<td>m'.m'</td>
<td>$0,1/2,0 [0,0,\bar{0}]$</td>
<td>$1/2,0,0 [0,0,\bar{0}]$</td>
<td>$1/2,0,0 [0,0,\bar{0}]$</td>
<td>$1/2,0,0 [0,0,\bar{0}]$</td>
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<tr>
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<td>---</td>
<td>---</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>4'/m'..</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>4'2'm'</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>1/2,0,1/4 [0,0,\bar{w}]</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>4'2'2</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p4'm'm</td>
<td>0,0,z</td>
</tr>
<tr>
<td></td>
<td>a* = (a - b)/2  b* = (a + b)/2</td>
<td></td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p_c'2mm</td>
<td>x,1/4,1/4</td>
</tr>
<tr>
<td></td>
<td>a* = b/2  b* = c/2</td>
<td></td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>p2m'm'</td>
<td>x,x,0</td>
</tr>
<tr>
<td></td>
<td>a* = (-a + b)/2  b* = c/2</td>
<td></td>
</tr>
</tbody>
</table>
I4/m'c'm'

140.9.1204

4/m'm'm'

I4/m'2/c'2/m'

Tetragonal

Origin at center (4/m') at 4/m'c'2/c'

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1 (1 | 0,0,0)

(2) 2 0,0,z (2z | 0,0,0)

(3) 4+ 0,0,z (4z | 0,0,0)

(4) 4- 0,0,z (4z⁻¹ | 0,0,0)

(5) 2 0,y,1/4 (2y | 0,0,1/2)

(6) 2 x,0,1/4 (2z | 0,0,1/2)

(7) 2 x,x,1/4 (2x | 0,0,1/2)

(8) 2 x,x,1/4 (2x | 0,0,1/2)

(9) 1' 0,0,0 (1 | 0,0,0)'

(10) m' x,y,0 (m | 0,0,0)'

(11) 4+ 0,0,z; 0,0,0 (4z | 0,0,0)'

(12) 4- 0,0,z; 0,0,0 (4z⁻¹ | 0,0,0)'

(13) c' (0,0,1/2) 0,y,z (m | 0,0,1/2)'

(14) c' (0,0,1/2) 0,y,z (m | 0,0,1/2)'

(15) c' (0,0,1/2) x,x,z (m | 0,0,1/2)'

(16) c' (0,0,1/2) x,x,z (m | 0,0,1/2)'

140.9.1204 - 1 - 2562
For \(1/2,1/2,1/2 \) + set

(1) \( t \) \((1/2,1/2,1/2) \)  \( (2) \) \((0,0,1/2) \) \((3) \) \( 4^* \) \((0,0,1/2) \) \((4) \) \( 4^* \) \((0,1/2) \)

(5) \( 2 \) \((0,1/2,0) \) \((6) \) \((1/2,0,0) \) \((7) \) \((1/2,1/2,0) \) \((8) \) \( x, x+1/2, 0 \)

(9) \( T \) \((1/2,1/2,1/2) \) \((10) \) \((1/2,1/2,1/2)' \) \((11) \) \((4)^* \) \((1/2,0, z) \) \((12) \) \((4)^* \) \((1/2,1/2,1/2)' \)

(13) \( a' \) \((1/2,0,0) \) \((14) \) \((0,1/2,0) \) \((15) \) \((1/2,1/2,0) \) \((16) \) \( x, x, z \)

Generators selected \((1); \) \((1,0,0); \) \((0,1,0); \) \((0,0,1); \) \((1/2,1/2,1/2); \) \((2); \) \((3); \) \((5); \) \((9).\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Wyckoff letter, Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 m 1</td>
<td>((1) x, y, z [u, v, w] )</td>
<td>((2) x, y, z [u, v, w] )</td>
<td>((3) y, x, z [v, u, w] )</td>
</tr>
<tr>
<td></td>
<td>((5) x, y, z+1/2 [u, v, w] )</td>
<td>((6) x, y, z+1/2 [u, v, w] )</td>
<td>((7) y, x, z+1/2 [v, u, w] )</td>
</tr>
<tr>
<td></td>
<td>((9) x, y, z [u, v, w] )</td>
<td>((10) x, y, z [u, v, w] )</td>
<td>((11) y, x, z [v, u, w] )</td>
</tr>
<tr>
<td></td>
<td>((13) x, y, z+1/2 [u, v, w] )</td>
<td>((14) x, y, z+1/2 [u, v, w] )</td>
<td>((15) y, x, z+1/2 [v, u, w] )</td>
</tr>
<tr>
<td></td>
<td>((16) x, x+1/2, z [u, u, w] )</td>
<td>((17) x, x+1/2, z [u, u, w] )</td>
<td>((18) x, x+1/2, z+1/2 [u, u, w] )</td>
</tr>
<tr>
<td></td>
<td>((19) x, x+1/2, z+1/2 [u, u, w] )</td>
<td>((20) x, x+1/2, z+1/2 [u, u, w] )</td>
<td>((21) x, x+1/2, z+1/2 [u, u, w] )</td>
</tr>
<tr>
<td>16 l ..m'..</td>
<td>((8) x, y, 0 [u, v, 0] )</td>
<td>((9) x, y, 0 [u, v, 0] )</td>
<td>((10) y, x, 0 [v, u, 0] )</td>
</tr>
<tr>
<td></td>
<td>((11) y, x, 1/2 [v, u, 0] )</td>
<td>((12) x, y, 1/2 [u, v, 0] )</td>
<td>((13) x, y, 1/2 [u, v, 0] )</td>
</tr>
<tr>
<td>16 j .2.</td>
<td>((14) x, 0, 1/4 [u, 0, 0] )</td>
<td>((15) x, 0, 1/4 [u, 0, 0] )</td>
<td>((16) x, 0, 1/4 [u, 0, 0] )</td>
</tr>
<tr>
<td></td>
<td>((17) x, 0, 3/4 [u, 0, 0] )</td>
<td>((18) x, 0, 3/4 [u, 0, 0] )</td>
<td>((19) x, 0, 3/4 [u, 0, 0] )</td>
</tr>
<tr>
<td>16 i .2</td>
<td>((20) x, x, 1/4 [u, u, 0] )</td>
<td>((21) x, x, 1/4 [u, u, 0] )</td>
<td>((22) x, x, 1/4 [u, u, 0] )</td>
</tr>
<tr>
<td></td>
<td>((23) x, x, 3/4 [u, u, 0] )</td>
<td>((24) x, x, 3/4 [u, u, 0] )</td>
<td>((25) x, x, 3/4 [u, u, 0] )</td>
</tr>
<tr>
<td>8 h m'.2m'</td>
<td>((26) x, x+1/2, 0 [u, u, 0] )</td>
<td>((27) x, x+1/2, 0 [u, u, 0] )</td>
<td>((28) x+1/2, x, 0 [u, u, 0] )</td>
</tr>
<tr>
<td>8 g 2.m'm'</td>
<td>((29) 0, 1/2, 0 [0, w] )</td>
<td>((30) 0, 1/2, 0 [0, w] )</td>
<td>((31) x, 1/2, z+1/2 [0, 0, w] )</td>
</tr>
<tr>
<td>8 f .4..</td>
<td>((32) 0, 0, z [0, w] )</td>
<td>((33) 0, 0, z [0, w] )</td>
<td>((34) 0, 0, z [0, w] )</td>
</tr>
<tr>
<td>8 e .2/m'</td>
<td>((35) 1/4, 1/4, 1/4 [0, 0, 0] )</td>
<td>((36) 1/4, 1/4, 1/4 [0, 0, 0] )</td>
<td>((37) 1/4, 3/4, 1/4 [0, 0, 0] )</td>
</tr>
<tr>
<td>4 d m'.m'm'</td>
<td>((38) 0, 1/2, 0 [0, 0, 0] )</td>
<td>((39) 1/2, 0, 0 [0, 0, 0] )</td>
<td>((40) 1/2, 0, 0 [0, 0, 0] )</td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>4/m' ..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>4</td>
<td>0,1/2,1/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>422</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

**Continued**

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'  
\[ \mathbf{a}^* = \frac{(\mathbf{a} - \mathbf{b})}{2} \quad \mathbf{b}^* = \frac{(\mathbf{a} + \mathbf{b})}{2} \]  
Origin at 0,0,z

Along [1,0,0] p2m'm'  
\[ \mathbf{a}^* = \frac{\mathbf{b}}{2} \quad \mathbf{b}^* = \frac{\mathbf{c}}{2} \]  
Origin at x,0,0

Along [1,1,0] p2m'm'  
\[ \mathbf{a}^* = \frac{(-\mathbf{a} + \mathbf{b})}{2} \quad \mathbf{b}^* = \frac{\mathbf{c}}{2} \]  
Origin at x,x,0
**Origin** at center (4/m) at 4/mc21/c

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y < 1/2 - x\]

**Symmetry Operations**

For (0,0,0) + set

1. \(1\) 1
   \(1\) 0,0,0
2. \(2\) \(0,0,z\)
   \(2\) 0,0,0
3. \(4\) \(0,0,z\)
   \(4\) 0,0,0
4. \(4\) \(0,0,z\)
   \(4\) 0,0,0
5. \(2\) \(0, y, 1/4\)
   \(2\) 0,0,1/2
6. \(2\) \(x, 0, 1/4\)
   \(2\) 0,0,1/2
7. \(2\) \(x, x, 1/4\)
   \(2\) 0,0,1/2
8. \(2\) \(x, x, 1/4\)
   \(2\) 0,0,1/2
9. \(3\) \(0,0,0\)
   \(3\) 0,0,0
10. \(m\) \(x, y, 0\)
    \(m\) 0,0,0
11. \(4\) \(0,0,z; 0,0,0\)
    \(4\) 0,0,0
12. \(4\) \(0,0,z; 0,0,0\)
    \(4\) 0,0,0
13. \(c\) \((0,0,1/2)\) \(x, 0, z\)
    \(c\) \((0,0,1/2)\) 0,0,1/2
14. \(c\) \((0,0,1/2)\) \(0, y, z\)
    \(c\) \((0,0,1/2)\) 0,0,1/2
15. \(c\) \((0,0,1/2)\) \(x, x, z\)
    \(c\) \((0,0,1/2)\) 0,0,1/2
16. \(c\) \((0,0,1/2)\) \(x, x, z\)
    \(c\) \((0,0,1/2)\) 0,0,1/2
Continued

For \((1/2,1/2,1/2)' + \text{ set}\)

<table>
<thead>
<tr>
<th>(1) \text{t}' (1/2,1/2,1/2)</th>
<th>(2) \text{t}' (0,0,1/2)</th>
<th>(3) \text{t}' (0,1/2,0)</th>
<th>(4) \text{t}' (0,0,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(5) \text{2}' (0,1/2,0)</th>
<th>(6) \text{2}' (1/2,0,0)</th>
<th>(7) \text{2}' (1/2,1/2,0)</th>
<th>(8) \text{2}' (1/2,1/2,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(9) \text{1}' (1/2,1/2,1/2)</th>
<th>(10) \text{1}' (0,1/2,0)</th>
<th>(11) \text{1}' (0,0,1/2)</th>
<th>(12) \text{1}' (0,0,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
<td>(1/2,1/2,1/2)'</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>(m 1)</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>16</td>
<td>(l \ldots m')</td>
<td>(x,y,z [u,v,w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(x+1/2,z [u,v,w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(+1/2,x,z [u,v,w])</td>
</tr>
<tr>
<td>8</td>
<td>(h m.2'm')</td>
<td>(x,x+1/2,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(x+1/2,0 [0,0,0])</td>
</tr>
<tr>
<td>8</td>
<td>(g 2.m'm')</td>
<td>(1/2,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(+1/2,z [0,0,0])</td>
</tr>
<tr>
<td>8</td>
<td>(f \ldots 4)</td>
<td>(0,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(+1/2,z [0,0,0])</td>
</tr>
<tr>
<td>4</td>
<td>(d m.m'm')</td>
<td>(0,1/2,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1/2,0 [0,0,0])</td>
</tr>
</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
</tr>
<tr>
<td>(1/2,1/2,1/2)</td>
</tr>
</tbody>
</table>

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Continued

| 4 | c | 4/m. | 0,0,0 [0,0,w] | 0,0,1/2 [0,0,w] |
| 4 | b | 4'2m' | 0,1/2,1/4 [0,0,0] | 1/2,0,1/4 [0,0,0] |
| 4 | a | 422 | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,0,0]</th>
<th>p22'2m'm'</th>
<th>Along [1,1,0]</th>
<th>p22'2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>a* = -c/2</td>
<td>b* = b/2</td>
<td>a* = -c/2</td>
<td>b* = (-a + b)/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
Origin at x,0,1/4
Origin at x,x,1/4
Origin at center (4/m') at 4/m'c2'/c

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

1. 1  
   (1 | 0,0,0)

2. 2  0,0,z  
   (2z | 0,0,0)

3. 4  0,0,z  
   (4z | 0,0,0)

4. 4' 0,0,z  
   (4'z | 0,0,0)

(1) 1  
   (1 | 0,0,0)

(2) 2  0,0,z  
   (2z | 0,0,0)

(3) 4  0,0,z  
   (4z | 0,0,0)

(4) 4' 0,0,z  
   (4'z | 0,0,0)

5. 2' 0,y,1/4  
   (2y | 0,0,1/2)'

6. 2' x,0,1/4  
   (2x | 0,0,1/2)'

7. 2' x,y,1/4  
   (2x | 0,0,1/2)'

8. 2' x,y,1/4  
   (2x | 0,0,1/2)'

(5) 2' 0,y,1/4  
   (2y | 0,0,1/2)'

(6) 2' x,0,1/4  
   (2x | 0,0,1/2)'

(7) 2' x,y,1/4  
   (2x | 0,0,1/2)'

(8) 2' x,y,1/4  
   (2x | 0,0,1/2)'

9. 1  0,0,0  
   (1 | 0,0,0)'

10. m' x,y,0  
    (mz | 0,0,0)'

11. 4' 0,0,z  
    (4'z | 0,0,0)'

12. 4' 0,0,z  
    (4'z | 0,0,0)'

(9) 1  0,0,0  
   (1 | 0,0,0)'

(10) m' x,y,0  
    (mz | 0,0,0)'

(11) 4' 0,0,z  
    (4'z | 0,0,0)'

(12) 4' 0,0,z  
    (4'z | 0,0,0)'

13. c (0,0,1/2) x,0,z  
    (my | 0,0,1/2)

14. c (0,0,1/2) 0,y,z  
    (my | 0,0,1/2)

15. c (0,0,1/2) x,y,z  
    (my | 0,0,1/2)

16. c (0,0,1/2) x,x,z  
    (my | 0,0,1/2)
Continued

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2)
(1/2,1/2,1/2)'
(2) 2' (0,0,1/2) 1/4,1/4,z
(2' 1/2,1/2,1/2)'
(3) 4' (0,0,1/2) 0,1/2,z
(4) 4' (0,0,1/2) 1/2,0,z
(4'_z' 1/2,1/2,1/2)'

(5) z (0,1/2,0) 1/4,y,0
(2_z 1/2,1/2,0)
(6) 2 (1/2,0,0) x,1/4,0
(2' 1/2,1/2,0)
(7) 2 (1/2,1/2,0) x,x,0
(2' 1/2,1/2,0)
(8) x,x+1/2,0
(2' 1/2,1/2,0)

(9) t' 1/4,1/4,1/4
(2' 1/2,1/2,1/2)
(10) n (1/2,1/2,0) x,y,1/4
(m_z 1/2,1/2,1/2)
(11) 4' 1/2,0,0; 1/2,0,1/4
(4') 1/2,1/2,1/2)
(12) 3' -0,1/2,0; 0,1/2,1/4
(3' -1/2,1/2,1/2)

(13) a' (1/2,0,0) x,1/4,z
(m_z 1/2,1/2,0)'
(14) b' (0,1/2,0) 1/4,y,z
(m_z 1/2,1/2,0)'
(15) m' x+1/2,x,z
(m_z 1/2,1/2,0)'
(16) g' (1/2,1/2,0) x,x,z
(m_z 1/2,1/2,0)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry letter.

Coordinates

(0,0,0) + (1/2,1/2,1/2)'

32 m 1
(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) y,x,z [v,u,w] (4) y,x,z [v,u,w]
(5) x,y,z+1/2 [u,v,w] (6) x,y,z+1/2 [u,v,w] (7) y,x,z+1/2 [v,u,w] (8) y,x,z+1/2 [v,u,w]
(9) x,y,z [u,v,w] (10) x,y,z [u,v,w] (11) y,x,z [v,u,w] (12) y,x,z [v,u,w]
(13) x,y,z+1/2 [u,v,w] (14) x,y,z+1/2 [u,v,w] (15) y,x,z+1/2 [v,u,w] (16) y,x,z+1/2 [v,u,w]

16 l ..m'
x,x,1/2,z [u,u,w] x,x,1/2,z [u,u,w] x+1/2,x,z [u,u,w] x+1/2,x,z [u,u,w]

16 k m''
x,y,0 [u,v,0] x,y,0 [u,v,0] y,x,0 [v,u,0] y,x,0 [v,u,0]

16 i ..2'
x,0,1/4 [0,v,w] x,0,1/4 [0,v,w] 0,x,1/4 [v,0,w] 0,x,1/4 [v,0,w]

16 h m'.2m'
x,x,1/2,0 [u,u,0] x,x,1/2,0 [u,u,0] x,1/2,x,0 [u,u,0] x+1/2,x,0 [u,u,0]

8 g 2.m''
0,1/2,0 [0,0,w] 1/2,0,0 [0,0,w] 0,1/2,0 [0,0,w] 1/2,0,0 [0,0,w]

8 f 4..
0,0,0 [0,0,w] 0,0,0 [0,0,w] 0,0,0 [0,0,w] 0,0,0 [0,0,w]

8 e ..2'm'
1/4,1/4,1/4 [u,u,w] 3/4,3/4,1/4 [u,u,w] 3/4,3/4,1/4 [u,u,w] 1/4,3/4,1/4 [u,u,w]

4 d m.m''
0,1/2,0 [0,0,w] 1/2,0,0 [0,0,w]
<table>
<thead>
<tr>
<th>4</th>
<th>c</th>
<th>4/m'..</th>
<th>0,0,0 [0,0,0]</th>
<th>0,0,1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>b</td>
<td>4'/2m'</td>
<td>0,1/2,1/4 [0,0,w]</td>
<td>1/2,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>42'2'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

| **Along [0,0,1]** | p
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>-c/2</td>
</tr>
<tr>
<td>b* = (a + b)/2</td>
<td>b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Along [1,0,0]</strong></th>
<th>p2a 2m' m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c/2</td>
<td>(a - b)/2</td>
</tr>
<tr>
<td>b* = b/2</td>
<td>(a + b)/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th><strong>Along [1,1,0]</strong></th>
<th>p2a 2m' m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = -c/2</td>
<td>(a - b)/2</td>
</tr>
<tr>
<td>b* = (a + b)/2</td>
<td>b/2</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Origin at center (4'/m) at 4'/mc'21/c

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y < 1/2 - x

Symmetry Operations

For (0,0,0) + set

1. (1) 1 (1 | 0,0,0)
2. (2) 2 0,0,z (2z | 0,0,0)
3. (3) 4+ 0,0,z (4z | 0,0,0)
4. (4) 4- 0,0,z (4z-1 | 0,0,0)

(5) 2' 0,y,1/4 (2z | 0,0,1/2)
6. (6) 2' x,0,1/4 (2z | 0,0,1/2)
7. (7) 2 x,x,1/4 (2xy | 0,0,1/2)
8. (8) 2 x,x,1/4 (2xy | 0,0,1/2)

(9) 1 0,0,0 (1 | 0,0,0)
10. (10) m x,y,0 (m | 0,0,0)
11. (11) 4' 0,0,z; 0,0,0 (4z | 0,0,0)
12. (12) 4' 0,0,z; 0,0,0 (4z-1 | 0,0,0)

(13) c' (0,0,1/2) x,0,z (m | 0,0,1/2)
14. (14) c' (0,0,1/2) 0,y,z (m | 0,0,1/2)
15. (15) c (0,0,1/2) x,x,z (mxy | 0,0,1/2)
16. (16) c (0,0,1/2) x,x,z (mxy | 0,0,1/2)
Continued

For \((1/2,1/2,1/2)' + \text{set}\)

\[
\begin{align*}
(1) & \ t' (1/2,1/2,1/2) \\
(1) & (1,1,1) \\
(2) & 2' (0,0,1/2) \\
(2) & 1/4,1/4,z \\
(3) & 4' (0,0,1/2) \\
(3) & 0,1/2,z \\
(4) & 4' (0,0,1/2) \\
(4) & 1/2,0,z \\
(5) & 2 (0,1/2,0) \\
(5) & 1/4,y,0 \\
(6) & 2 (1/2,0,0) \\
(6) & x,1/4,0 \\
(7) & 2' (1/2,1/2,0) \\
(7) & x,x,0 \\
(8) & 2' x,x +1/2,0 \\
(8) & (2,1/2,1/2)' \\
(9) & \tilde{T} 1/4,1/4,1/4 \\
(9) & x,y,1/4 \\
(10) & 4' (1/2,0,0,z; 1/2,0,1/4) \\
(10) & (4,1/2,1/2,1/2)' \\
(11) & 4' (0,1/2,0; 1/2,1,1/2) \\
(11) & (4,0,1/2,1/2)' \\
(12) & 4' 0,1/2,z; 0,1/2,1/4 \\
(12) & (4,0,1/2,1/2)' \\
(13) & a (1/2,0,0) x,1/4,z \\
(13) & (m,1/2,1/2,0) x,y,1/4,0 \\
(14) & b (0,1/2,0) 1/4,y,z \\
(14) & (m,1/2,1/2,0) x,x,0 \\
(15) & m' x+1/2,x,z \\
(15) & (m_{xy},1/2,1/2,0)' \\
(16) & g' (1/2,1/2,0) x,x,z \\
(16) & (m_{xy},1/2,1/2,0)' \\
\end{align*}
\]

**Generators selected**

\(1); \ t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ t'(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter, Site Symmetry</th>
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<tr>
<td>32</td>
<td>m 1</td>
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<tr>
<td>16</td>
<td>l .m'</td>
</tr>
<tr>
<td>16</td>
<td>k m..</td>
</tr>
<tr>
<td>8</td>
<td>h m.2'm'</td>
</tr>
<tr>
<td>8</td>
<td>g 2.m'm'</td>
</tr>
<tr>
<td>8</td>
<td>f 4'..</td>
</tr>
<tr>
<td>8</td>
<td>e .2/m'</td>
</tr>
<tr>
<td>4</td>
<td>d m.m'm'</td>
</tr>
</tbody>
</table>

**Coordinates**

\[
\begin{align*}
(0,0,0) + & \\
(1/2,1/2,1/2)' + & \\
\end{align*}
\]

<table>
<thead>
<tr>
<th>(x,y,z[u,v,w])</th>
<th>(x,y,z[u,v,w])</th>
<th>(y,x,z[v,u,w])</th>
<th>(y,x,z[v,u,w])</th>
<th>(y,x,z[v,u,w])</th>
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</thead>
<tbody>
<tr>
<td>(x,y,0[0,0,w])</td>
<td>(x,y,0[0,0,w])</td>
<td>(y,x,0[0,0,w])</td>
<td>(y,x,0[0,0,w])</td>
<td>(y,x,0[0,0,w])</td>
</tr>
<tr>
<td>(x,y,1/2[0,0,w])</td>
<td>(x,y,1/2[0,0,w])</td>
<td>(y,x,1/2[0,0,w])</td>
<td>(y,x,1/2[0,0,w])</td>
<td>(y,x,1/2[0,0,w])</td>
</tr>
<tr>
<td>(x,0,1/4[0,v,w])</td>
<td>(x,0,1/4[0,v,w])</td>
<td>(0,x,1/4[0,v,w])</td>
<td>(0,x,1/4[0,v,w])</td>
<td>(0,x,1/4[0,v,w])</td>
</tr>
<tr>
<td>(x,0,3/4[0,v,w])</td>
<td>(x,0,3/4[0,v,w])</td>
<td>(0,x,3/4[0,v,w])</td>
<td>(0,x,3/4[0,v,w])</td>
<td>(0,x,3/4[0,v,w])</td>
</tr>
<tr>
<td>(x,1/4[u,u,0])</td>
<td>(x,1/4[u,u,0])</td>
<td>(x,1/4[u,u,0])</td>
<td>(x,1/4[u,u,0])</td>
<td>(x,1/4[u,u,0])</td>
</tr>
<tr>
<td>(x,1/4[u,u,0])</td>
<td>(x,3/4[u,u,0])</td>
<td>(x,3/4[u,u,0])</td>
<td>(x,3/4[u,u,0])</td>
<td>(x,3/4[u,u,0])</td>
</tr>
<tr>
<td>(x,x+1/2[0,0,w])</td>
<td>(x,x+1/2[0,0,w])</td>
<td>(x+1/2,x,0[0,0,w])</td>
<td>(x+1/2,x,0[0,0,w])</td>
<td>(x+1/2,x,0[0,0,w])</td>
</tr>
<tr>
<td>(x,2,z[0,0,w])</td>
<td>(x,2,z[0,0,w])</td>
<td>(0,1/2,z+1/2[0,0,w])</td>
<td>(0,1/2,z+1/2[0,0,w])</td>
<td>(0,1/2,z+1/2[0,0,w])</td>
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<tr>
<td>(x,2,0[0,0,w])</td>
<td>(x,2,0[0,0,w])</td>
<td>(0,0,z+1/2[0,0,0])</td>
<td>(0,0,z+1/2[0,0,0])</td>
<td>(0,0,z+1/2[0,0,0])</td>
</tr>
<tr>
<td>(x,2,1/4[0,0,0])</td>
<td>(x,2,1/4[0,0,0])</td>
<td>(3/4,3/4,1/4[0,0,0])</td>
<td>(3/4,3/4,1/4[0,0,0])</td>
<td>(3/4,3/4,1/4[0,0,0])</td>
</tr>
<tr>
<td>(x,2,0[0,0,w])</td>
<td>(x,2,0[0,0,w])</td>
<td>(1/2,0,0[0,0,w])</td>
<td>(1/2,0,0[0,0,w])</td>
<td>(1/2,0,0[0,0,w])</td>
</tr>
</tbody>
</table>
4 c 4′/m.. 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]
4 b 4′2′m′ 0,1/2,1/4 [0,0,w] 1/2,0,1/4 [0,0, w]
4 a 4′2′2 0,0,1/4 [0,0,0] 0,0,3/4 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p4mm1′
\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \]
\[ \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]
Origin at 0,0,z

Along [1,0,0] p2a* 2mm
\[ \mathbf{a}^* = \mathbf{b}/2 \]
\[ \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x,1/4,0

Along [1,1,0] p2a* 2m′m′
\[ \mathbf{a}^* = -\mathbf{c}/2 \]
\[ \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]
Origin at x,x,1/4
**Origin** at center (4'/m) at 4'/mc2'/c'

**Asymmetric unit**

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y \leq 1/2 - x
\]

**Symmetry Operations**

For (0,0,0) + set

1. \((1)\ 1\ (1 \ 0,0,0)\)
2. \((2)\ 2\ 0,0,z\ (2_z,0,0,0)\)
3. \((3)\ 4'\ 0,0,z\ (4_z,0,0,0)'\)
4. \((4)\ 4'\ 0,0,z\ (4_z,0,0,0)'\)
5. \((5)\ 2\ 0,y,1/4\ (2_y,0,0,1/2)\)
6. \((6)\ 2\ x,0,1/4\ (2_z,0,0,1/2)\)
7. \((7)\ 2'\ x,x,1/4\ (2_{xy},0,0,1/2)'\)
8. \((8)\ 2'\ x,\bar{x},1/4\ (2_{xy},0,0,1/2)'\)
9. \((9)\ \bar{1}\ 0,0,0\ (1 \ 0,0,0)\)
10. \((10)\ m\ x,y,0\ (m_z,0,0,0)\)
11. \((11)\ 4''\ 0,0,z; 0,0,0\ (4_z,0,0,0)'\)
12. \((12)\ 4''\ 0,0,z; 0,0,0\ (4_z,0,0,0)'\)
13. \((13)\ c\ (0,0,1/2)\ x,0,z\ (m_y,0,0,1/2)\)
14. \((14)\ c\ (0,0,1/2)\ 0,y,z\ (m_z,0,0,1/2)\)
15. \((15)\ c'\ (0,0,1/2)\ x,\bar{x},z\ (m_{xy},0,0,1/2)'\)
16. \((16)\ c'\ (0,0,1/2)\ x,x,z\ (m_{xy},0,0,1/2)'\)
For \((1/2,1/2,1/2)'+\) + set

\[
\begin{align*}
(1) & \ t' (1/2,1/2,1/2) \\
(2) & \ 2' (0,0,1/2) 1/4,1/4,z \\
(3) & \ 4' (0,0,1/2) 0,1/2,z \\
(4) & \ 4' (0,0,1/2) 1/2,0,z \\
(5) & \ 2' (0,1/2,0) 1/4,y,0 \\
(6) & \ 2' (1/2,0,0) 0,y,z \\
(7) & \ 2' (1/2,0,0) x,z \\
(8) & \ 2' (0,0,1/2) 1/2,0,z \\
(9) & \ y,x+1/2,0 \\
(10) & \ x,y,z+1/2 [u,v,w] \\
(11) & \ y,x,z+1/2 [u,v,w] \\
(12) & \ y,x,z+1/2 [u,v,w] \\
(13) & \ a' (1/2,0,0) x,y,z+1/2 [u,v,w] \\
(14) & \ b' (0,1/2,0) x,y,z+1/2 [u,v,w] \\
(15) & \ g (1/2,1/2,0) x,y,z+1/2 [u,v,w] \\
(16) & \ g (1/2,1/2,0) x,y,z+1/2 [u,v,w] \\
\end{align*}
\]

Generators selected 
\((1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).\)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generators</td>
<td>((0,0,0) + (1/2,1/2,1/2)' + (1/2,1/2,1/2))</td>
</tr>
<tr>
<td>((1)) x,y,z [u,v,w]</td>
<td>((2)) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>((3)) y,x,z [v,u,w]</td>
<td>((4)) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>((5)) x,y,z+1/2 [u,v,w]</td>
<td>((6)) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>((7)) y,x,z+1/2 [v,u,w]</td>
<td>((8)) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>((9)) x,y,z [u,v,w]</td>
<td>((10)) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>((11)) x,y,z [v,u,w]</td>
<td>((12)) x,y,z [v,u,w]</td>
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<tr>
<td>((13)) x,y,z+1/2 [u,v,w]</td>
<td>((14)) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td>((15)) x,y,z+1/2 [v,u,w]</td>
<td>((16)) x,y,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>((16)) x,y,z+1/2 [u,v,w]</td>
<td>((17)) x,y,z+1/2 [u,v,w]</td>
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</table>

<table>
<thead>
<tr>
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<th>Coordinates</th>
</tr>
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<tbody>
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<td>((16)) m.. x,y,0 [0,0,w]</td>
<td>((16)) m.. x,y,0 [0,0,w]</td>
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<tr>
<td>((16)) x,y,1/2 [0,0,w]</td>
<td>((16)) x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>((16)) x,0,1/4 [u,0,0]</td>
<td>((16)) x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td>((16)) x,0,3/4 [u,0,0]</td>
<td>((16)) x,0,3/4 [u,0,0]</td>
</tr>
<tr>
<td>((16)) x,0,1/4 [u,0,0]</td>
<td>((16)) x,0,1/4 [u,0,0]</td>
</tr>
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<td>((8)) x,x,1/4 [u,0,0]</td>
<td>((8)) x,x,1/4 [u,0,0]</td>
</tr>
<tr>
<td>((8)) x,x,3/4 [u,0,0]</td>
<td>((8)) x,x,3/4 [u,0,0]</td>
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<table>
<thead>
<tr>
<th>Generators</th>
<th>Coordinates</th>
</tr>
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<tbody>
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<td>((8)) m.2m x,x+1/2,0 [0,0,0]</td>
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<tr>
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<td>((8)) m.2m x,x+1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along \([0,0,1]\) p4mm1' 
\[a^* = (a - b)/2 \quad b^* = (a + b)/2\]
Origin at 0,0,z

Along \([1,0,0]\) p_{22}m'm' 
\[a^* = b/2 \quad b^* = c/2\]
Origin at x,0,1/4

Along \([1,1,0]\) p2mm1' 
\[a^* = (-a + b)/2 \quad b^* = c/2\]
Origin at x,x,0
Origin at center (4'/m') at 4'/m'c'2'/c

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1
   (1|0,0,0)

(5) 2 0,y,1/4
    (2_y|0,0,1/2)

(9) 1' 0,0,0
    (1|0,0,0)'

(13) c' (0,0,1/2) x,0,z
     (m_x|0,0,1/2)'

(2) 2 0,0,z
    (2_z|0,0,0)

(6) 2 x,0,1/4
    (2_x|0,0,1/2)

(10) m' x,y,0
     (m_z|0,0,0)'

(14) c' (0,0,1/2) 0,y,z
     (m_y|0,0,1/2)'

(3) 4+ 0,0,z
    (4_z|0,0,0)'

(7) 2' x,x,1/4
    (2_x|0,0,1/2)'

(11) 4+ 0,0,z; 0,0,0
     (4_z|0,0,0)

(12) 4- 0,0,z; 0,0,0
     (4_z^-1|0,0,0)

(4) 4- 0,0,z
    (4_z^-1|0,0,0)'

(8) 2' x,x,1/4
    (2_x|0,0,1/2)'

(15) c (0,0,1/2) x,x,z
     (m_y|0,0,1/2)

(16) c (0,0,1/2) x,x,z
     (m_y|0,0,1/2)
Continued

For \((1/2,1/2,1/2)' + \text{ set}\)

<table>
<thead>
<tr>
<th>(m)</th>
<th>(l)</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
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<tr>
<td></td>
<td></td>
<td>(<del>x',y',z'</del>[u',v',w]~)</td>
</tr>
<tr>
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<td></td>
<td>(<del>y',x',z'</del>[v',u,w]~)</td>
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<tr>
<td></td>
<td></td>
<td>(<del>y',x,z</del>[v,u,w]~)</td>
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<tr>
<td>16</td>
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<td>(<del>x,x+1/2,z</del>[u,u,w]~)</td>
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<td>(<del>x+x+1/2,z</del>[u,u,w]~)</td>
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<td>16</td>
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<td>(<del>x,y,0</del>[u,v,0]~)</td>
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<td>j</td>
<td>(<del>x,x+1/4</del>[u,u,w]~)</td>
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<td>g</td>
<td>(<del>0,1/2,z</del>[0,0,w]~)</td>
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<td>(<del>0,0,z</del>[0,0,0]~)</td>
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<td>8</td>
<td>e</td>
<td>(<del>1/4,1/4,1/4</del>[u,v,0]~)</td>
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<tr>
<td></td>
<td></td>
<td>(<del>3/4,3/4,1/4</del>[u,v,0]~)</td>
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<td></td>
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<td>(<del>3/4,3/4,1/4</del>[v,u,0]~)</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>(<del>0,1/2,0</del>[0,0,0]~)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(<del>1/2,0,0</del>[0,0,0]~)</td>
</tr>
</tbody>
</table>

**Generators selected**

(1); \((1,0,0)\); \((0,1,0)\); \((0,0,1)\); \((1/2,1/2,1/2)\); (2); (3); (5); (9).
4  c  4'/m'..  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]
4  b  4'2m'  0,1/2,1/4 [0,0,0]  1/2,0,1/4 [0,0,0]
4  a  4'22'  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  \( p_{c'} \cdot 4m'm' \)  
\( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  
Origin at 0,1/2,z

Along [1,0,0]  \( p_{2a'} \cdot 2m'm' \)  
\( a^* = b/2 \)  \( b^* = c/2 \)  
Origin at x,0,0

Along [1,1,0]  \( p_{2a'} \cdot 2m'm' \)  
\( a^* = -c/2 \)  \( b^* = (-a + b)/2 \)  
Origin at x,x,0
Origin at center (4/m) at 4/mc'2'/c'

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ 1/2 - x

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2z) 0,0,0

(3) 4⁺ 0,0,z
(4z) 0,0,0

(4) 4⁻ 0,0,z
(4z⁻¹) 0,0,0

(5) 2’ 0,y,1/4
(2y) 0,0,1/2’

(6) 2’ x,0,1/4
(2x) 0,0,1/2’

(7) 2’ x,x,1/4
(2xx) 0,0,1/2’

(8) 2’ x,x,1/4
(2x) 0,0,1/2’

(9) 1 0,0,0
(1) 0,0,0

(10) m x,y,0
(m) 0,0,0

(11) 4⁺ 0,0,z; 0,0,0
(4x) 0,0,0

(12) 4⁻ 0,0,z; 0,0,0
(4x⁻¹) 0,0,0

(13) c’ (0,0,1/2) x,0,z
(m) 0,0,1/2’

(14) c’ (0,0,1/2) 0,y,z
(m) 0,0,1/2’

(15) c’ (0,0,1/2) x,x,z
(m) 0,0,1/2’

(16) c’ (0,0,1/2) x,x,z
(m) 0,0,1/2’
For $(1/2,1/2,1/2)' + \text{set}$

(1) $t'(1/2,1/2,1/2)$
(2) $2'(0,0,1/2) 1/4,1/4,z$
(3) $4^{+},' (0,0,1/2) 0,1/2,z$
(4) $4^{+} (0,0,1/2) 1/2,0,z$
(5) $2 (0,1/2,0) 1/4,y,0$
(6) $2 (0,1/2,0) 1/4,y,0$
(7) $2 (0,1/2,0) x,x,0$
(8) $2 x, x+1/2,0$
(9) $1/4,1/4,1/4$ $x,y,0$
(10) $1/4,1/4,1/4$ $x,y,0$
(11) $1/4,1/4,1/4$ $x,y,0$
(12) $1/4,1/4,1/4$ $x,y,0$
(13) $a (1/2,0,0) x,1/4,z$
(14) $b (0,1/2,0) 1/4,y,z$
(15) $m x+1/2,x,1/4$
(16) $g (1/2,1/2,0) x,x,z$

Generators selected (1); $t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9).$

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m$</td>
<td>$x,y,z [u,v,w]$</td>
</tr>
<tr>
<td>$m$</td>
<td>$x,y,z [u,v,w]$</td>
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<td>$m$</td>
<td>$x,y,z [u,v,w]$</td>
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<td>$x,y,z [u,v,w]$</td>
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<td>$x,y,z [u,v,w]$</td>
</tr>
<tr>
<td>$m$</td>
<td>$x,y,z [u,v,w]$</td>
</tr>
</tbody>
</table>

16 $l$  $..m$

16 $k$  $m..$

16 $j$  $..2'$

16 $i$  $..2'$

8 $h$  $m.2m$

8 $g$  $2.mm$

8 $f$  $4.$

8 $e$  $..2'/m$

4 $d$  $m.mm$

140.15.1210 - 2 - 2581
4  c  4/m..  0,0,0 [0,0,w]  0,0,1/2 [0,0,w]
4  b  4'2'm  0,1/2,1/4 [0,0,0]  1/2,0,1/4 [0,0,0]
4  a  42'2'  0,0,1/4 [0,0,w]  0,0,3/4 [0,0,w]

Symmetry of Special Projections

Along [0,0,1]  p4mm1'  
\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]  
Origin at 0,0,z

Along [1,0,0]  p2a*2mm  
\[ \mathbf{a}^* = \mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{b}/2 \]  
Origin at x,1/4,0

Along [1,1,0]  p2mm1'  
\[ \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]  
Origin at x,x,0
**Origin** at center (4/m’<sup>1</sup>) at 4/m’c2,/c’

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y \leq 1/2 - x \]

**Symmetry Operations**

For (0,0,0) + set

1. \(1\) origin
2. \(2\) \((0,0,z)\)\((0,0,0)\)
3. \(2'\) \((0,0,1/2)\)
4. \(2'\) \((0,0,1/2)\)
5. \(2'\) \((0,0,1/2)\)
6. \(2'\) \((0,0,1/2)\)
7. \(2'\) \((0,0,1/2)\)
8. \(2'\) \((0,0,1/2)\)
9. \(\mathbf{m}'\) \((0,0,0)\)
10. \(\mathbf{m}'\) \((0,0,0)\)
11. \(\mathbf{m}'\) \((0,0,0)\)
12. \(\mathbf{m}'\) \((0,0,0)\)
13. \(\mathbf{m}'\) \((0,0,0)\)
14. \(\mathbf{m}'\) \((0,0,0)\)
15. \(\mathbf{m}'\) \((0,0,0)\)
16. \(\mathbf{m}'\) \((0,0,0)\)
Continued

For $(1/2,1/2,1/2)' + \text{set}$

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(1) $t'(1/2,1/2,1/2)$</td>
<td>$(0,0,0) + (1/2,1/2,1/2)' +$</td>
</tr>
<tr>
<td>(2) $2'(0,0,1/2)$</td>
<td>$1/4,1/4,z$</td>
</tr>
<tr>
<td>(3) $4^+ (0,0,1/2)$</td>
<td>$0,1/2,z$</td>
</tr>
<tr>
<td>(4) $2'(0,1/2,0)$</td>
<td>$1/2,0,z$</td>
</tr>
<tr>
<td>(5) $x'(0,1/2,0)$</td>
<td>$1/4,y,0$</td>
</tr>
<tr>
<td>(6) $2'(0,1/2,0)$</td>
<td>$x,1/4,0$</td>
</tr>
<tr>
<td>(7) $2'(1/2,1/2,0)$</td>
<td>$x,x,0$</td>
</tr>
<tr>
<td>(8) $2' x,x+1/2,0$</td>
<td>$(2_{xy})$</td>
</tr>
<tr>
<td>(9) $1/4,1/4,1/4$</td>
<td>$(m_{zy})$</td>
</tr>
<tr>
<td>(10) $n(1/2,1/2,0)$</td>
<td>$x,y,1/4$</td>
</tr>
<tr>
<td>(11) $4^+(1/2,0,0); z; 1/2,0,1/4$</td>
<td>$(4z)$</td>
</tr>
<tr>
<td>(12) $4^+ (1/2,1/2,1/2)'$</td>
<td>$(4z)$</td>
</tr>
<tr>
<td>(13) $a'(1/2,0,0)$</td>
<td>$x,1/4,z$</td>
</tr>
<tr>
<td>(m_{zy})</td>
<td>$(1/2,1/2,0)'$</td>
</tr>
<tr>
<td>(14) $b'(0,1/2,0)$</td>
<td>$1/4,y,z$</td>
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<tr>
<td>(m_{zy})</td>
<td>$(1/2,1/2,0)'$</td>
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<tr>
<td>(15) $m x+1/2,x,z$</td>
<td>$(mx)$</td>
</tr>
<tr>
<td>(16) $g (1/2,1/2,0)$</td>
<td>$x,x,z$</td>
</tr>
</tbody>
</table>

**Generators selected**

(1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t'(1/2,1/2,1/2)$; (2); (3); (5); (9).

**Positions**

*Multiplicity, Wyckoff letter, Site Symmetry letter.*

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<thead>
<tr>
<th>m</th>
<th>32</th>
<th>1</th>
<th>(1) $x,y,z [u,v,w]$</th>
<th>(2) $x,y,z [u,v,w]$</th>
<th>(3) $y,x,z [v,u,w]$</th>
<th>(4) $y,x,z [v,u,w]$</th>
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</thead>
<tbody>
<tr>
<td>l</td>
<td>16</td>
<td>m'..</td>
<td>$x,y,0 [u,v,0]$</td>
<td>$x,y,0 [u,v,0]$</td>
<td>$y,x,0 [v,u,0]$</td>
<td>$y,x,0 [v,u,0]$</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>j ..2'.</td>
<td>$x,0,1/4 [0,v,w]$</td>
<td>$x,0,1/4 [0,v,w]$</td>
<td>$0,x,1/4 [v,0,w]$</td>
<td>$0,x,1/4 [v,0,w]$</td>
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<td>16</td>
<td>i ..2</td>
<td>$x,x,1/4 [u,u,0]$</td>
<td>$x,x,1/4 [u,u,0]$</td>
<td>$x,x,1/4 [u,u,0]$</td>
<td>$x,x,1/4 [u,u,0]$</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>h m'..2'm</td>
<td>$x,x+1/2,0 [u,u,0]$</td>
<td>$x,x+1/2,0 [u,u,0]$</td>
<td>$x+1/2,x,0 [u,u,0]$</td>
<td>$x+1/2,x,0 [u,u,0]$</td>
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<tr>
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<td>8</td>
<td>g 2.mm</td>
<td>$0,1/2,z [0,0,0]$</td>
<td>$1/2,0,z [0,0,0]$</td>
<td>$0,1/2,z+1/2 [0,0,0]$</td>
<td>$1/2,0,z+1/2 [0,0,0]$</td>
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<tr>
<td></td>
<td>8</td>
<td>f 4'. ..</td>
<td>$0,0,z [0,0,0]$</td>
<td>$0,0,z [0,0,0]$</td>
<td>$0,0,z [0,0,0]$</td>
<td>$0,0,z [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>e ..2/m</td>
<td>$1/4,1/4,1/4 [0,0,0]$</td>
<td>$3/4,3/4,1/4 [0,0,0]$</td>
<td>$3/4,3/4,1/4 [0,0,0]$</td>
<td>$1/4,3/4,1/4 [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>d m'.mm</td>
<td>$0,1/2,0 [0,0,0]$</td>
<td>$1/2,0,0 [0,0,0]$</td>
<td>$1/2,0,0 [0,0,0]$</td>
<td>$1/2,0,0 [0,0,0]$</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1]  \( p_{4mm} \)
\[
a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2}
\]
Origin at 0,0,z

Along [1,0,0]  \( p_{2m'm'} \)
\[
a^* = -\frac{c}{2} \quad b^* = \frac{b}{2}
\]
Origin at x,0,0

Along [1,1,0]  \( p_{2mm1'} \)
\[
a^* = -\frac{a + b}{2} \quad b^* = \frac{c}{2}
\]
Origin at x,x,0
Tetragonal

140.17.1212

\[ \text{Origin at center } (4/m') \text{ at } 4/m'c'2/c'/c' \]

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y < 1/2 - x \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \quad (1|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \quad (2_2|0,0,0) \\
(3) & \quad 4^+ \quad 0,0,z \quad (4_2|0,0,0) \\
(4) & \quad 4^- \quad 0,0,z \quad (4_2^-|0,0,0) \\
(5) & \quad 2 \quad 0,y,1/4 \quad (2_y|0,0,1/2) \\
(6) & \quad 2 \quad x,0,1/4 \quad (2_x|0,0,1/2) \\
(7) & \quad 2 \quad x,x,1/4 \quad (2_{xy}|0,0,1/2) \\
(8) & \quad 2 \quad x,x,1/4 \quad (2_{xy}|0,0,1/2) \\
(9) & \quad \bar{1} \quad 0,0,0 \quad (1|0,0,0)' \\
(10) & \quad m' \quad x,y,0 \quad (m_x|0,0,0)' \\
(11) & \quad \bar{4}^+ \quad 0,0,z; 0,0,0 \quad (4_2|0,0,0)' \\
(12) & \quad \bar{4}^- \quad 0,0,z; 0,0,0 \quad (4_2^-|0,0,0)' \\
(13) & \quad c' \quad (0,0,1/2) \quad x,0,z \quad (m_y|0,0,1/2)' \\
(14) & \quad c' \quad (0,0,1/2) \quad 0,y,z \quad (m_y|0,0,1/2)' \\
(15) & \quad c' \quad (0,0,1/2) \quad x,x,z \quad (m_{xy}|0,0,1/2)' \\
(16) & \quad c' \quad (0,0,1/2) \quad x,x,z \quad (m_{xy}|0,0,1/2)' \\
\end{align*}
\]
For $(1/2,1/2,1/2)' + \text{ set}$

$(1) \ t'(1/2,1/2,1/2)$

$(2) 2'(0,0,1/2) 1/4,1/4,z$

$(3) 4' (0,0,1/2) 0,1/2,z$

$(4) 4' (0,0,1/2) 1/2,0,z$

$(5) 2'(0,1/2,0) 1/4,y,0$

$(6) 2'(1/2,0,0) x,1/4,0$

$(7) 2'(1/2,1/2,0) x,x,0$

$(8) 2' x,x+1/2,0$

$(9) \ T 1/4,1/4,1/4$

$(10) n (1/2,1/2,0) x,y,1/4$

$(11) 4' (1/2,1/2,0) 1/2,0,1/4$

$(12) 4' (1/2,1/2,0) 0,1/2,z$

$(13) a (1/2,0,0) x,1/4,z$

$(14) b (0,1/2,0) 1/4,y,z$

$(15) m x+1/2,x,z$

$(16) g (1/2,1/2,0) x,x,z$

**Generators selected**

(1); $t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (9)$.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinate(s)</th>
</tr>
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<tbody>
<tr>
<td>32 m 1</td>
<td>$x,y,z [u,v,w]$</td>
</tr>
<tr>
<td></td>
<td>$(1/2,1/2,1/2)' +$</td>
</tr>
<tr>
<td>16 l .m</td>
<td>$x,x+1/2,z [u,u,0]$</td>
</tr>
<tr>
<td></td>
<td>$x+1/2,x,z [u,u,0]$</td>
</tr>
<tr>
<td>16 k m'.2</td>
<td>$x,y,0 [u,v,0]$</td>
</tr>
<tr>
<td></td>
<td>$x,y,0 [u,v,0]$</td>
</tr>
<tr>
<td>16 j .2</td>
<td>$x,0,1/4 [u,0,0]$</td>
</tr>
<tr>
<td></td>
<td>$0,x,1/4 [u,0,0]$</td>
</tr>
<tr>
<td>16 i .2</td>
<td>$x,x,1/4 [u,u,0]$</td>
</tr>
<tr>
<td></td>
<td>$x,x,1/4 [u,u,0]$</td>
</tr>
<tr>
<td>8 h m'.2$m</td>
<td>$x,x+1/2,0 [u,u,0]$</td>
</tr>
<tr>
<td></td>
<td>$x+1/2,x,0 [u,u,0]$</td>
</tr>
<tr>
<td>8 g 2.mm</td>
<td>$0,1/2,z [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td>$1/2,0,z [0,0,0]$</td>
</tr>
<tr>
<td>8 f 4..</td>
<td>$0,0,z [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$0,0,z [0,0,w]$</td>
</tr>
<tr>
<td>8 e .2/m</td>
<td>$1/4,1/4,1/4 [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$3/4,1/4,1/4 [0,0,w]$</td>
</tr>
<tr>
<td>4 d m'.mm</td>
<td>$0,1/2,0 [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td>$1/2,0,0 [0,0,0]$</td>
</tr>
</tbody>
</table>
4  c  4/m'..  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]
4  b  2/m  0,1/2,1/4 [0,0,0]  1/2,0,1/4 [0,0,0]
4  a  422  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p_4'  4m'm'
\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]
Origin at 0,0,z

Along [1,0,0]  p_{2a'}  2m'm'
\[ \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x,0,0

Along [1,1,0]  p_{2mm1'}
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x,x,0
Origin at $\overline{4}m2$ at $0,1/4,1/8$ from center (2/m)

Asymmetric unit

\[ 0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/8 \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \quad (1,0,0,0) \\
(2) & \quad 2 \quad 0,0,z \quad (2_z,0,0,0) \\
(3) & \quad 4^+ \quad (0,0,1/4) \quad -1/4,1/4,z \quad (4_z,0,1/2,1/4) \\
(4) & \quad 4^- \quad (0,0,1/4) \quad 1/4,1/4,z \quad (4_z^{-1},0,1/2,1/4) \\
(5) & \quad 2 \quad (0,1/2,0) \quad 0,y,1/8 \quad (2_y,0,1/2,1/4) \\
(6) & \quad 2 \quad x,1/4,1/8 \quad (2_x,0,1/2,1/4) \\
(7) & \quad 2 \quad x,x,0 \quad (2_{xx},0,0,0) \\
(8) & \quad 2 \quad x,x,0 \quad (2_{xx},0,0,0) \\
(9) & \quad \overline{1} \quad 0,1/4,1/8 \quad (1,0,1/2,1/4) \\
(10) & \quad b \quad (0,1/2,0) \quad x,y,1/8 \quad (m_y,0,1/2,1/4) \\
(11) & \quad \overline{4}^+ \quad 0,0,z; 0,0,0 \quad (4_z,0,0,0) \\
(12) & \quad \overline{4}^- \quad 0,0,z; 0,0,0 \quad (4_z^{-1},0,0,0) \\
(13) & \quad m \quad x,0,z \quad (m_x,0,0,0) \\
(14) & \quad m \quad 0,y,z \quad (m_y,0,0,0) \\
(15) & \quad d \quad (-1/4,1/4,1/4) \quad x+1/4,\overline{x},z \quad (m_{xy},0,1/2,1/4) \\
(16) & \quad d \quad (1/4,1/4,1/4) \quad x-1/4,\overline{x},z \quad (m_{xy},0,1/2,1/4)
\end{align*}
\]
For \((1/2,1/2,1/2) + \) set

1. \(t(1/2,1/2,1/2)
2. \(2(0,0,1/2)\)
3. \(4^+(0,0,3/4)\)
4. \(4^-(0,0,3/4)\)

(1) \(t(1/2,1/2,1/2)\)
(2) \(2(0,0,1/2)\)
(3) \(4^+(0,0,3/4)\)
(4) \(4^-(0,0,3/4)\)

Generators selected

1; \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(1/2,1/2,1/2)\); (2); (3); (5); (9).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>(i)</td>
<td>(1)</td>
</tr>
<tr>
<td>16</td>
<td>(h)</td>
<td>(0.0,0))</td>
</tr>
<tr>
<td>16</td>
<td>(g)</td>
<td>(0.0,1/2)z+1/4)</td>
</tr>
<tr>
<td>16</td>
<td>(f)</td>
<td>(x,1/4,1/8)</td>
</tr>
<tr>
<td>8</td>
<td>(e)</td>
<td>(0,0,z)</td>
</tr>
<tr>
<td>8</td>
<td>(d)</td>
<td>(0,1/4,5/8)</td>
</tr>
<tr>
<td>8</td>
<td>(c)</td>
<td>(0,1/4,1/8)</td>
</tr>
</tbody>
</table>

### Coordinates

- \((0,0,0) + (1/2,1/2,1/2) + (1,0,0)\)

- \(x,y,z\) \([u,v,w]\)
- \(y,y,z\) \([u,v,w]\)
- \(y,y,z\) \([u,v,w]\)
- \(x,y+1/2,z+1/4\) \([u,v,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)
- \(x,y+1/2,z+1/4\) \([u,v,w]\)
- \(y,x,z\) \([v,u,w]\)
- \(x,y,z\) \([v,u,w]\)
- \(x,y,z\) \([v,u,w]\)
- \(x,y+1/2,z+1/4\) \([v,u,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)
- \(y,x+1/2,z+1/4\) \([v,u,w]\)

### Generators

- \(1\); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(1/2,1/2,1/2)\); (2); (3); (5); (9).
Symmetry of Special Projections

Along [0,0,1] \( p_{\parallel} \) 4m'\( m' \)
\( a^* = a/2 \quad b^* = b/2 \)
Origin at 1/4,1/4,z

Along [1,0,0] c2mm1'
\( a^* = b \quad b^* = c \)
Origin at x,0,3/8

Along [1,1,0] \( c_{p'} \) 2m'\( m' \)
\( a^* = (-a + b)/2 \quad b^* = c/2 \)
Origin at x,x,0
Origin at $\overline{4}m2$ at 0,1/4,-1/8 from center (2/m)

Asymmetric unit: $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
   $(1 | 0,0,0)$

2. $2$
   $(0,0,z) (2_z|0,0,0)$

3. $4^+$
   $(0,0,1/4) -1/4,1/4,z (4_z|0,1/2,1/4)$

4. $4^-$
   $(0,0,1/4) 1/4,1/4,z (4_z^{-1}|0,1/2,1/4)$

5. $2$
   $(0,1/2,0) 0,y,1/8 (2_y|0,1/2,1/4)$

6. $2$
   $x,1/4,1/8 (2_z|0,1/2,1/4)$

7. $2$
   $x,x,0 (2_{xy}|0,0,0)$

8. $2$
   $x,x,0 (2_{xy}|0,0,0)$

9. $\overline{1}$
   $0,1/4,1/8 (\bar{1}|0,1/2,1/4)$

10. $b$
    $(0,1/2,0) x,y,1/8 (m_{xy}|0,1/2,1/4)$

11. $\overline{4}^+$
    $0,0,z; 0,0,0 (\bar{4}_z|0,0,0)$

12. $\overline{4}^-$
    $0,0,z; 0,0,0 (\bar{4}_z^{-1}|0,0,0)$

13. $m$
    $x,0,z (m_{x}|0,0,0)$

14. $m$
    $0,y,z (m_y|0,0,0)$

15. $d$
    $(-1/4,1/4,1/4) x+1/4,\bar{x},z (m_{xy}|0,1/2,1/4)$

16. $d$
    $(1/4,1/4,1/4) x-1/4,\bar{x},z (m_{xy}|0,1/2,1/4)$
Generators selected  
(1): (1,0,0); (0,1,0); (0,0,1); (1/2,1,2,1/2); (2); (3); (5); (9); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
</table>

Continued 141.2.1214  

For (1/2,1/2,1/2) + set

<table>
<thead>
<tr>
<th>(1) t (1/2,1/2,1/2)</th>
<th>(2) 2 (0,0,1/2)</th>
<th>1/4,1/4,z (3) 4' (0,0,3/4)</th>
<th>1/4,1/4,z (4) 4' (0,0,3/4)</th>
<th>1/4,-1/4,z (4') 1/2,0,3/4</th>
<th>1/2,0,3/4</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>(1) t (1/2,1/2,1/2)</th>
<th>(2) 2 (0,0,1/2)</th>
<th>1/4,1/4,z (3) 4' (0,0,3/4)</th>
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<th>1/4,-1/4,z (4') 1/2,0,3/4</th>
<th>1/2,0,3/4</th>
</tr>
</thead>
</table>

For (0,0,0) + set

<table>
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<tr>
<th>(1) t (1/2,1/2,1/2)</th>
<th>(2) 2 (0,0,1/2)</th>
<th>1/4,1/4,z (3) 4' (0,0,3/4)</th>
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<th>1/4,-1/4,z (4') 1/2,0,3/4</th>
<th>1/2,0,3/4</th>
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</table>

For (1/2,1,2,1/2) + set

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<tr>
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<th>(2) 2' (0,0,1/2)</th>
<th>1/4,1/4,z (3) 4' (0,0,3/4)</th>
<th>1/4,1/4,z (4) 4' (0,0,3/4)</th>
<th>1/4,-1/4,z (4') 1/2,0,3/4</th>
<th>1/2,0,3/4</th>
</tr>
</thead>
</table>

141.2.1214 - 2 - 2593
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Operation</th>
<th>Symmetry</th>
<th>Origin</th>
<th>a*</th>
<th>b*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4mm1'</td>
<td>0,0,0</td>
<td>a/2</td>
<td>b/2</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>c2mm1'</td>
<td>0,0,0</td>
<td>b</td>
<td>c</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>c2mm1'</td>
<td>x,x,0</td>
<td>(-a + b)/2</td>
<td>c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

#### 32 i 11'

<table>
<thead>
<tr>
<th>Transformation</th>
<th>Notation</th>
<th>Origin</th>
<th>a</th>
<th>b</th>
<th>c</th>
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<tbody>
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<td>(1) x,y,z</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>(2) x,y,z</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3) y,x+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>y,x,z</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4) y,x+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>y,x,z</td>
<td>[0,0,0]</td>
<td></td>
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</tr>
<tr>
<td>(5) x,y+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
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</tr>
<tr>
<td>(6) x,y+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
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<tr>
<td>(7) y,x,z</td>
<td>[0,0,0]</td>
<td>y,x,z</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(8) y,x,z</td>
<td>[0,0,0]</td>
<td>y,x,z</td>
<td>[0,0,0]</td>
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<tr>
<td>(9) x,y+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
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<tr>
<td>(10) x,y+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(11) y,x,z</td>
<td>[0,0,0]</td>
<td>y,x,z</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(12) y,x,z</td>
<td>[0,0,0]</td>
<td>y,x,z</td>
<td>[0,0,0]</td>
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</tr>
<tr>
<td>(13) x,y,z</td>
<td>[0,0,0]</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
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<tr>
<td>(14) x,y,z</td>
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<td>x,y,z</td>
<td>[0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(15) y,x+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>y,x+1/2,z+1/4</td>
<td>[0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>(16) y,x+1/2,z+1/4</td>
<td>[0,0,0]</td>
<td>y,x+1/2,z+1/4</td>
<td>[0,0,0]</td>
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### Symmetry of Special Projections

<table>
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<td>0,0,0</td>
<td>a/2</td>
<td>b/2</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>c2mm1'</td>
<td>0,0,0</td>
<td>b</td>
<td>c</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>c2mm1'</td>
<td>x,x,0</td>
<td>(-a + b)/2</td>
<td>c/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
Origin at $\overline{4}m2'$ at 0,1/4,-1/8 from center ($2'm$)

Asymmetric unit

$0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1
(1 0,0,0)

(5) $2' (0,1/2,0) \ 0,y,1/8$
($2'_y | 0,1/2,1/4)'

(9) $\overline{1}' 0,1/4,1/8$
($\overline{1} | 0,1/2,1/4)'

(13) m $x,0,z$
($m_y | 0,0,0)$

(2) $2 \ 0,0,z$
($2_z | 0,0,0)$

(6) $2' \ x,1/4,1/8$
($2_z | 0,1/2,1/4)'

(10) $b' (0,1/2,0) \ x,y,1/8$
($m_y | 0,1/2,1/4)'

(14) m $0,y,z$
($m_y | 0,0,0)$

(3) $4^+ (0,0,1/4) \ -1/4,1/4,z$
($4_z | 0,1/2,1/4)$

(7) $2' \ x,x,0$
($2_{xy} | 0,0,0)'$

(11) $\overline{4}^\prime \ 0,0,z; 0,0,0$
($\overline{4}_z | 0,0,0)'$

(15) d $(-1/4,1/4,1/4) \ 1/4, x,z$
($m_{xy} | 0,1/2,1/4)$

(16) d $(1/4,1/4,1/4) \ -x,1/4,x,z$
($m_{xy} | 0,1/2,1/4)$
Continued

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1); t(1,0,0); t(0,1,0); t(1/2,2,1/2); (2); (3); (5); (9).</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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</table>

### Positions

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<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>32 i 1</td>
<td>x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>32</td>
<td>y,x+1/2,z+1/4 [v,u,w]</td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>32</td>
<td>x,y+1/2,z+1/4 [u,v,w]</td>
<td>(6) x,y+1/2,z+1/4 [u,v,w]</td>
</tr>
<tr>
<td>32</td>
<td>y,x,z [v,u,w]</td>
<td>(8) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>32</td>
<td>x,y+1/2,z+1/4 [u,v,w]</td>
<td>(10) x,y+1/2,z+1/4 [u,v,w]</td>
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<td>32</td>
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</tbody>
</table>

| 16 h .m. | 0,y,z [u,0,0] 0,y,z [u,0,0] | 0,y,z [u,0,0] |
| 16 | 0,y+1/2,z+1/4 [u,0,0] 0,y+1/2,z+1/4 [u,0,0] | 0,y+1/2,z+1/4 [u,0,0] |
| 16 | x,x,0 [u,u,w] x,x,0 [u,u,w] | x,x,0 [u,u,w] |
| 16 | x,x+1/2,1/4 [u,u,w] x,x+1/2,1/4 [u,u,w] | x,x+1/2,1/4 [u,u,w] |
| 16 | x,1/4,1/8 [0,v,w] x,3/4,1/8 [0,v,w] | 3/4,x+1/2,3/8 [0,v,0,w] |
| 16 | x,1/4,1/8 [0,v,w] x,3/4,1/8 [0,v,w] | 1/4,x,7/8 [v,0,w] |
| 16 | 0,0,z [0,0,0] 0,1/2,z+1/4 [0,0,0] | 0,0,z [0,0,0] |
| 8 e 2mm. | 0,1/4,5/8 [0,0,0] 0,3/4,5/8 [0,0,0] | 0,1/4,2,7/8 [0,0,0] |
| 8 d .2/m'. | 0,1/4,1/8 [0,0,0] 0,3/4,1/8 [0,0,0] | 0,1/4,2,3/8 [0,0,0] |
| 8 c .2/m'. | 0,1/4,1/8 [0,0,0] 0,3/4,1/8 [0,0,0] | 0,1/4,2,3/8 [0,0,0] |

141.3.1215 - 2 - 2596
4  b  \( \overline{4}2'm \)  0,0,1/2 [0,0,0]  0,1/2,3/4 [0,0,0]
4  a  \( \overline{4}2'm \)  0,0,0 [0,0,0]  0,1/2,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4mm  \( a^* = a/2 \)  \( b^* = b/2 \)
Origin at 0,0,z

Along [1,0,0]  c2mm1'  \( a^* = b \)  \( b^* = c \)
Origin at x,0,3/8

Along [1,1,0]  \( c_p' \)  2'mm'  \( a^* = -c/2 \)  \( b^* = (-a + b)/2 \)
Origin at x,x,0
I4₁/am'd
141.4.1216

4'/mm'm
I4₁/a2'/m'2/d

Tetragonal

Origin at \( \overline{2}m'2 \) at 0,1/4,-1/8 from center (2'/m')

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/8

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(5) 2' (0,1/2,0) 0,y,1/8
 (2', 0,1/2,1/4')

(9) \( \overline{1} \) 0,1/4,1/8
 (\( \overline{1} \) | 0,1/2,1/4)

(13) m' x,0,z
 (m', 0,0,0)'

(2) 2 0,0,z
 (2z, 0,0,0)

(6) 2' x,1/4,1/8
 (2z, 0,1/2,1/4)'

(10) b (0,1/2,0) x,y,1/8
 (m, 0,1/2,1/4)

(14) m' 0,y,z
 (m', 0,0,0)'

(3) 4⁺ (0,0,1/4) -1/4,1/4,z
 (4z, 0,1/2,1/4)'

(7) 2 x,x,0
 (2z, 0,0,0)

(8) 2 x,x,0
 (2z, 0,0,0)

(4) 4⁻ (0,0,1/4) 1/4,1/4,z
 (4z⁻¹, 0,1/2,1/4)'

(11) 4⁻ (0,0,1/4) 0,z; 0,0,0
 (4z⁻¹, 0,0,0)'

(12) 4⁻ (0,0,1/4) 0,z; 0,0,0
 (4z⁻¹, 0,0,0)'

(15) d (-1/4,1/4,1/4) x+1/4,x,z
 (m, 0,1/2,1/4)

(16) d (1/4,1/4,1/4) x-1/4,x,z
 (m, 0,1/2,1/4)
Generators selected  
(1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<td>32</td>
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<tr>
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<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td>(1/2,1/2,1/2)</td>
<td>(3)</td>
<td>y,x+1/2,z+1/4 [v,u,w]</td>
<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
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<td>x,y+1/2,z+1/4 [u,v,w]</td>
<td>(6) x,y+1/2,z+1/4 [u,v,w]</td>
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<td>y,x+1/2 [v,u,w]</td>
<td>(8) y,x+1/2 [v,u,w]</td>
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<td>(1/2,1/2,1/2)</td>
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<td>.m'</td>
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<tr>
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<td>0,y,z [0,v,w]</td>
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<td>0,y+1/2,z+1/4 [0,v,w]</td>
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<tr>
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<td>0,y,0 [v,w]</td>
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<td>x,x,0 [u,u,u]</td>
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<td>x,x+1/2,1/4 [u,u,u]</td>
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<tr>
<td>(1/2,1/2,1/2)</td>
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<td>0,1/2,z+1/4 [0,0,0]</td>
<td>0,1/2,z+1/4 [0,0,0]</td>
</tr>
<tr>
<td>(1/2,1/2,1/2)</td>
<td>(4)</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>(1/2,1/2,1/2)</td>
<td>(5)</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<tr>
<td>(1/2,1/2,1/2)</td>
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<td>0,0,z [0,0,0]</td>
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</table>
4 b $\text{4‘2‘m}$ 0,0,1/2 [0,0,0] 0,1/2,3/4 [0,0,0]
4 a $\text{4‘2‘m}$ 0,0,0 [0,0,0] 0,1/2,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p$_{\text{c}$, 4mm
a* = a/2 b* = b/2
Origin at 0,0,z

Along [1,0,0] c2m‘m‘

a* = b b* = c
Origin at x,0,3/8

Along [1,1,0] c$_{\text{p‘}$ 2m‘m‘

a* = (-a + b)/2 b* = c/2
Origin at x,x,0
Origin at $\overline{4}m2'$ at 0,1/4,-1/8 from center (2/m)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) +$ set

(1) 1

(2) $\overline{4}' (0,0,1/4); -1/4,1/4,z$

(3) $4' (0,0,1/4); -1/4,1/4,z$

(4) $4' (0,0,1/4); 1/4,1/4,z$

(5) $2 (0,1/2,0); 0,y,1/8$

(6) $x,1/4,1/8$

(7) $2' x,x,0$

(8) $2' x,x,0$

(9) $\overline{1} 0,1/4,1/8$

(10) $b (0,1/2,0); x,y,1/8$

(11) $\overline{4}'; 0,0,z; 0,0,0$

(12) $\overline{4}'; 0,0,z; 0,0,0$

(13) $m x,0,z$

(14) $m 0,y,z$

(15) $d' (-1/4,1/4,1/4) \overline{x+1/4, \overline{x},z}$

(16) $d'(1/4,1/4,1/4) \overline{x-1/4, x,z}$
For \((1/2,1/2,1/2) + \) set

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<th>(1) t</th>
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<tr>
<td>(2) 2</td>
<td>0,0,1/2</td>
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<tr>
<td>(3) 4'</td>
<td>(0,0,3/4)</td>
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<tr>
<td>(4) 4'</td>
<td>(0,0,3/4)</td>
</tr>
<tr>
<td>(5) 2</td>
<td>1/2,0,3/4</td>
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<td>(6) 2</td>
<td>0,0,1/2</td>
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<tr>
<td>(7) 2'</td>
<td>(1/2,1/2,0)</td>
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<td>(8) 2'</td>
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</table>

Generators selected: 
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

### Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
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<td>x,y+1/2,z+1/4 [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
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<td>y,x,z [v,u,w]</td>
<td>(4) y,x,z [v,u,w]</td>
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<td>x,y+1/2,z+1/4 [u,v,w]</td>
<td>(5) x,y,z [v,u,w]</td>
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<td>(9) x,y,z [v,u,w]</td>
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<td>(13) x,y,z [u,v,w]</td>
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<td>y,z [u,0,0]</td>
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<td>y,z [u,0,0]</td>
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<td>x,0 [u,u,w]</td>
<td>(21) x,0 [u,u,w]</td>
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<td>8 e 2mm.</td>
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<td>0,0,z [0,0,0]</td>
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Coordinates:

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Continued

4 b $\bar{4}2m'$ 0,0,1/2 [0,0,0] 0,1/2,3/4 [0,0,0]
4 a $\bar{4}2m'$ 0,0,0 [0,0,0] 0,1/2,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p$_{\bar{4}m}$ 4mm
a* = a/2 b* = b/2
Origin at 0,0,z

Along [1,0,0] c2mm1'
a* = b b* = c
Origin at x,0,3/8

Along [1,1,0] c2'mm'
a* = -c/2 b* = (-a + b)/2
Origin at x,x,0
Origin at $\overline{4}m'2'$ at $0,1/4,-1/8$ from center ($2/m'$)

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
2. $2' \quad x,1/4,1/8$
3. $4' \quad (0,0,1/4) \rightarrow -1/4,1/4,z$
4. $4' \quad (0,0,1/4) \rightarrow 1/4,1/4,z$
5. $2 \quad (0,1/2,0) \rightarrow 0,y,1/8$
6. $2' \quad x,x,0$
7. $2' \quad x,x,0$
8. $2' \quad x,x,0$
9. $1' \quad 0,1/4,1/8$
10. $b' \quad (0,1/2,0) \rightarrow x,y,1/8$
11. $4' \quad 0,0,z; 0,0,0$
12. $4' \quad 0,0,z; 0,0,0$
13. $m' \quad x,0,z$
14. $m' \quad 0,y,z$
15. $d \quad (-1/4,1/4,1/4) \rightarrow x+1/4,\overline{x},z$
16. $d \quad (1/4,1/4,1/4) \rightarrow x-1/4,\overline{x},z$
For (1/2,1/2,1/2) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
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<td>(.m')</td>
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<tr>
<td>4</td>
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<td>(d)</td>
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<tr>
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<tr>
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<td>(y,z) [v,u,w]</td>
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<td>(.m')</td>
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<td>9</td>
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<td>14</td>
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<td>(d)</td>
<td>.2'm'</td>
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<td>(.m')</td>
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<td>16</td>
<td>(y,x+1/2,z+1/4) [v,u,w]</td>
<td>16</td>
<td>(.m')</td>
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Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).
4 b 42m 0,0,1/2 [0,0,0] 0,1/2,3/4 [0,0,0]
4 a 42m 0,0,0 [0,0,0] 0,1/2,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p, 4m'm'
\[ a^* = a/2 \quad b^* = b/2 \]
Origin at 0,0,z

Along [1,0,0] c2m'm'
\[ a^* = b \quad b^* = c \]
Origin at x,0,3/8

Along [1,1,0] c, 2mm'
\[ a^* = -c/2 \quad b^* = (-a + b)/2 \]
Origin at x,x,0
**Origin** at 4\text{m'2'} at 0,1/4,-1/8 from center (2'/m' )

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \(1 \quad 0,0,0 \)
2. \(2 \quad 0,0,z \)
3. \(4^+ \quad (0,0,1/4) \quad -1/4,1/4,z \)
4. \(4^+ \quad (0,0,1/4) \quad 1/4,1/4,z \)
5. \(2' \quad (0,1/2,0) \quad x,1/4,1/8 \)
6. \(2' \quad x,1/4,1/8 \)
7. \(2' \quad x,x,0 \)
8. \(2' \quad x,x,0 \)
9. \(m' \quad x,0,z \)
10. \(m' \quad 0,y,z \)
11. \(d' \quad -1/4,1/4,1/4 \quad x+1/4,x,z \)
12. \(d' \quad -1/4,1/4,1/4 \quad x-1/4,x,z \)
For (1/2,1/2,1/2) + set

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<tr>
<td>(3) ( \bar{y},x+1/2,z+1/4 [\bar{v},u,w] )</td>
<td>(4) ( y,x+1/2,z+1/4 [v,u,w] )</td>
</tr>
<tr>
<td>(5) ( \bar{x},y+1/2,z+1/4 [u,\bar{v},w] )</td>
<td>(6) ( x,\bar{y}+1/2,z+1/4 [u,v,w] )</td>
</tr>
<tr>
<td>(7) ( y,\bar{x},z [\bar{v},\bar{u},w] )</td>
<td>(8) ( \bar{y},\bar{x},z [v,u,w] )</td>
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<tr>
<td>(9) ( \bar{x},\bar{y}+1/2,z+1/4 [u,v,w] )</td>
<td>(10) ( x,y+1/2,\bar{z}+1/4 [\bar{u},\bar{v},w] )</td>
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<td>(11) ( y,\bar{x},\bar{z} [\bar{v},\bar{u},w] )</td>
<td>(12) ( \bar{y},x,\bar{z} [v,u,w] )</td>
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<tr>
<td>(13) ( x,y,z [u,v,w] )</td>
<td>(14) ( x,y,z [u,v,w] )</td>
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<td>(15) ( \bar{y},x+1/2,z+1/4 [\bar{v},\bar{u},w] )</td>
<td>(16) ( y,x+1/2,z+1/4 [v,u,w] )</td>
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<table>
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<th>16</th>
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<td>(0,y,z [0,v,w])</td>
<td>(0,( \bar{y},z [0,\bar{v},w] ))</td>
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<tr>
<td>0,y+1/4,z+1/2 [0,v,w]</td>
<td>( \bar{y},1/2,z+1/4 [\bar{v},0,w] ))</td>
</tr>
<tr>
<td>( y,1/2,z+1/4 [v,0,w] )</td>
<td>( y,0,z [v,0,w] )</td>
</tr>
<tr>
<td>0,( \bar{y},+1/2,z+1/4 [\bar{v},0,w] )</td>
<td>0,( \bar{y},0,z [\bar{v},0,w] )</td>
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<td>16</td>
<td>g .2'</td>
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<td>-----------------</td>
<td>----------------</td>
</tr>
<tr>
<td>(x,x,0 [\bar{u},\bar{u},w])</td>
<td>(( \bar{x},\bar{x},0 [u,u,w] ))</td>
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<td>( \bar{x},x,0 [u,u,w] )</td>
<td>( \bar{x},\bar{x}+1/2,1/4 [u,u,w] )</td>
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<tr>
<td>( x,\bar{x}+1/2,1/4 [u,u,w] )</td>
<td>( x,\bar{x}+1/2,1/4 [u,u,w] )</td>
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<td>16</td>
<td>f .2'</td>
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<tr>
<td>-----------------</td>
<td>----------------</td>
</tr>
<tr>
<td>(x,1/4,1/8 [0,v,w])</td>
<td>(x,3/4,1/8 [0,\bar{v},w])</td>
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<tr>
<td>3/4,x+1/2,3/8 [\bar{v},0,w]</td>
<td>1/4,( \bar{x},1/2,3/8 [v,0,w] )</td>
</tr>
<tr>
<td>1/4,( \bar{x},1/2,3/8 [v,0,w] )</td>
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</tr>
<tr>
<td>8</td>
<td>e 2m'm'</td>
</tr>
<tr>
<td>-----------------</td>
<td>----------------</td>
</tr>
<tr>
<td>(0,0,z [0,0,w])</td>
<td>(0,( 1/2,z+1/4 [0,0,w] ))</td>
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<tr>
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<td>( 0,0,z [0,0,w] )</td>
</tr>
<tr>
<td>8</td>
<td>d .2'm'</td>
</tr>
<tr>
<td>-----------------</td>
<td>----------------</td>
</tr>
<tr>
<td>(0,1/4,5/8 [0,0,w])</td>
<td>(0,3/4,5/8 [0,0,w])</td>
</tr>
<tr>
<td>3/4,1/2,7/8 [0,0,w]</td>
<td>1/4,( 1/2,7/8 [0,0,w] )</td>
</tr>
<tr>
<td>1/4,( 1/2,7/8 [0,0,w] )</td>
<td>3/4,( 1/2,3/8 [0,0,w] )</td>
</tr>
<tr>
<td>8</td>
<td>c .2'm'</td>
</tr>
<tr>
<td>-----------------</td>
<td>----------------</td>
</tr>
<tr>
<td>(0,1/4,1/8 [0,0,w])</td>
<td>(0,3/4,1/8 [0,0,w])</td>
</tr>
<tr>
<td>3/4,1/2,3/8 [0,0,w]</td>
<td>1/4,( 1/2,3/8 [0,0,w] )</td>
</tr>
<tr>
<td>141.7.1219 - 2 - 2608</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] \( p_{m} \) \( 4m'm' \)  
\( a^* = a/2 \quad b^* = b/2 \)  
Origin at 1/4,1/4,z

Along [1,0,0] \( c_{2}mm' \)  
\( a^* = -c \quad b^* = b \)  
Origin at x,0,3/8

Along [1,1,0] \( c_{2}mm' \)  
\( a^* = -c/2 \quad b^* = (-a + b)/2 \)  
Origin at x,x,0
**Origin**

at \( \overline{4} m 2 \) at 0,1/4,-1/8 from center (2'/m )

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8 \]

**Symmetry Operations**

For \((0,0,0) + \) set

1. \( 1 \)
   \( \begin{align*} 
   & (1|0,0,0) \\
   
   & (2) \begin{array}{c} \begin{pmatrix} z \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \end{array} \begin{pmatrix} 0 \end{pmatrix} \\
   \end{align*} \)

2. \( 2 \begin{pmatrix} 0,0,0 \end{pmatrix} \)
   \( \begin{align*} 
   & (2) \begin{pmatrix} z \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \end{align*} \)

3. \( 4^+ \begin{pmatrix} 0,0,1/4 \end{pmatrix} \begin{pmatrix} -1/4,1/4,1/4 \end{pmatrix} \)
   \( \begin{align*} 
   & (4) \begin{pmatrix} 0,1/1/2,1/4 \end{pmatrix} \\
   \begin{pmatrix} z \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \end{align*} \)

4. \( 4^- \begin{pmatrix} 0,0,1/4 \end{pmatrix} \begin{pmatrix} 1/4,1/4,1/4 \end{pmatrix} \)
   \( \begin{align*} 
   & (4) \begin{pmatrix} 0,1/1/2,1/4 \end{pmatrix} \\
   \begin{pmatrix} z \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \end{align*} \)

5. \( 2' \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} 0,y,1/8 \end{pmatrix} \)
   \( \begin{align*} 
   & (2) \begin{pmatrix} x \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \begin{pmatrix} 1/4 \end{pmatrix} \\
   \end{align*} \)

6. \( 2' \begin{pmatrix} x,1/4,1/8 \end{pmatrix} \begin{pmatrix} 1/2,1/4 \end{pmatrix} \)
   \( \begin{align*} 
   & (2) \begin{pmatrix} x \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \begin{pmatrix} 1/4 \end{pmatrix} \\
   \end{align*} \)

7. \( 2' \begin{pmatrix} x,x,0 \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} \)
   \( \begin{align*} 
   & (2) \begin{pmatrix} x \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \end{align*} \)

8. \( 2' \begin{pmatrix} x,x,0 \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} \)
   \( \begin{align*} 
   & (2) \begin{pmatrix} x \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \end{align*} \)

9. \( \overline{1} \begin{pmatrix} 0,1/4,1/8 \end{pmatrix} \begin{pmatrix} 0,1/2,1/4 \end{pmatrix} \)
   \( \begin{align*} 
   & (10) b' \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} x,y,1/8 \end{pmatrix} \)
   \begin{align*} 
   & (m) \begin{pmatrix} z \end{pmatrix} \\
   \begin{pmatrix} 0 \end{pmatrix} \\
   \begin{pmatrix} 1/2 \end{pmatrix} \\
   \end{align*} \)

10. \( b' \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} x,y,1/8 \end{pmatrix} \)
    \( \begin{align*} 
    & (m) \begin{pmatrix} z \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \begin{pmatrix} 1/2 \end{pmatrix} \\
    \end{align*} \)

11. \( \overline{4}^+ \begin{pmatrix} 0,0,1/2 \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} \)
    \( \begin{align*} 
    & (4) \begin{pmatrix} 0,0,0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \end{align*} \)

12. \( \overline{4}^- \begin{pmatrix} 0,0,1/2 \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} \)
    \( \begin{align*} 
    & (4) \begin{pmatrix} 0,0,0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \end{align*} \)

13. \( m \begin{pmatrix} x,0,z \end{pmatrix} \begin{pmatrix} m \end{pmatrix} \)
    \( \begin{align*} 
    & (m) \begin{pmatrix} 0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \end{align*} \)

14. \( m \begin{pmatrix} 0,y,z \end{pmatrix} \begin{pmatrix} m \end{pmatrix} \)
    \( \begin{align*} 
    & (m) \begin{pmatrix} 0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \end{align*} \)

15. \( d' \begin{pmatrix} -1/4,1/4,1/4 \end{pmatrix} \begin{pmatrix} x+1/4,x,z \end{pmatrix} \)
    \( \begin{align*} 
    & (4) \begin{pmatrix} 0,1/2,1/4 \end{pmatrix} \\
    \begin{pmatrix} m \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \end{align*} \)

16. \( d' \begin{pmatrix} 1/4,1/4,1/4 \end{pmatrix} \begin{pmatrix} x-1/4,x,z \end{pmatrix} \)
    \( \begin{align*} 
    & (4) \begin{pmatrix} 0,1/2,1/4 \end{pmatrix} \\
    \begin{pmatrix} m \end{pmatrix} \\
    \begin{pmatrix} 0 \end{pmatrix} \\
    \end{align*} \)
Continued

For (1/2,1/2,1/2) + set

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<tr>
<th>(1) t (1/2,1/2,1/2)</th>
<th>(2) 2 (0,0,1/2) 1/4,1/4,z</th>
<th>(3) 4' (0,0,3/4) 1/4,1/4,z</th>
<th>(4) 4' (0,0,3/4) 1/4,-1/4,z</th>
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<td>(2z, 1/2,1/2,1/2)</td>
<td>(4z, 1/2,0,3/4)</td>
<td>(4z, 1/2,0,3/4)</td>
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(5) 2' 1/4,y,3/8
  (2z, 1/2,0,3/4)'
(6) 2' (1/2,0,0) x,0,3/8
  (2z, 1/2,0,3/4)'
(7) (1/2,1/2,0) x,x,1/4
  (2z, 1/2,1/2,1/2)
(8) 2 x,x+1/2,1/4
  (2z, 1/2,1/2,1/2)

(9) 1/2,0,3/4)
  (1/2,0,3/4)'
(10) a' (1/2,0,0) x,y,3/8
    (mz, 1/2,0,3/4)'
(11) 4' 1/2,0,1/4 z,1/2,0,1/4
    (4z, 1/2,1/2,1/2)
(12) 4' 0,1/2,z; 0,1/2,1/4
    (4z, 1/2,1/2,1/2)

(13) n (1/2,0,1/2) x,1/4,z
    (mz, 1/2,1/2,1/2)
(14) n (0,1/2,1/2) 1/4,y,z
    (mz, 1/2,1/2,1/2)
(15) d' (1/4,-1/4,3/4) x+1/4,x
    (mz, 1/2,0,3/4)'
(16) d'(1/4,1/4,3/4) x+1/4,x,z
    (mz, 1/2,1/2,1/2)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

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<th>Positions</th>
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<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
<td>(3) y,x+1/2,z+1/4 [v,u,w]</td>
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<td>(4) y,x+1/2,z+1/4 [v,u,w]</td>
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<td>(5) x,y+1/2,z+1/4 [u,v,w]</td>
<td>(5) x,y+1/2,z+1/4 [u,v,w]</td>
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<td>(6) x,y+1/2,z+1/4 [u,v,w]</td>
<td>(6) x,y+1/2,z+1/4 [u,v,w]</td>
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<tr>
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<td>(7) y,x,z [v,u,w]</td>
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<td>(8) y,x,z [v,u,w]</td>
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<td>(9) x,y+1/2,z+1/4 [u,v,w]</td>
<td>(9) x,y+1/2,z+1/4 [u,v,w]</td>
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<tr>
<td></td>
<td>(10) x,y+1/2,z+1/4 [u,v,w]</td>
<td>(10) x,y+1/2,z+1/4 [u,v,w]</td>
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<td>(11) y,x,z [v,u,w]</td>
<td>(11) y,x,z [v,u,w]</td>
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<td>(12) y,x,z [v,u,w]</td>
<td>(12) y,x,z [v,u,w]</td>
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<td>(13) x,y,z [u,v,w]</td>
<td>(13) x,y,z [u,v,w]</td>
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<td>(14) x,y,z [u,v,w]</td>
<td>(14) x,y,z [u,v,w]</td>
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<td>(15) y,x+1/2,z+1/4 [v,u,w]</td>
<td>(15) y,x+1/2,z+1/4 [v,u,w]</td>
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<td>(16) y,x+1/2,z+1/4 [v,u,w]</td>
<td>(16) y,x+1/2,z+1/4 [v,u,w]</td>
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</table>

16 h .m. 0,y,z [u,0,0] 0,y,z [u,0,0] y,1/2,z+1/4 [0,u,0] y,1/2,z+1/4 [0,u,0]
0,y+1/2,z+1/4 [u,0,0] 0,y+1/2,z+1/4 [u,0,0] y,0,z [0,u,0] y,0,z [0,u,0]
16 g .2 x,x,0 [u,u,0] x,x,0 [u,u,0] x,x+1/2,1/4 [u,u,0] x,x+1/2,1/4 [u,u,0]
- x,x+1/2,1/4 [u,u,0] x,x+1/2,1/4 [u,u,0] x,x,0 [u,u,0] x,x,0 [u,u,0]
16 f .2' x,1/4,1/8 [0,v,w] x,3/4,1/8 [0,v,w] 3/4,x+1/2,3/8 [v,0,w] 1/4,x+1/2,3/8 [v,0,w]
 x,1/4,1/8 [0,v,w] x,3/4,1/8 [0,v,w] 3/4,x+1/2,3/8 [v,0,w] 1/4,x+1/2,3/8 [v,0,w]
8 e 2mm. 0,0,z [0,0,0] 0,1/2,z+1/4 [0,0,0] 0,1/2,z+1/4 [0,0,0] 0,0,z [0,0,0]
8 d .2'/m. 0,1/4,5/8 [0,0,0] 0,3/4,5/8 [0,0,0] 3/4,1/2,7/8 [0,0,0] 1/4,1/2,7/8 [0,0,0]
8 c .2'/m. 0,1/4,1/8 [0,0,0] 0,3/4,1/8 [0,0,0] 3/4,1/2,3/8 [0,0,0] 1/4,1/2,3/8 [0,0,0]
Symmetry of Special Projections

Along [0,0,1] p4'm'  
\(a^* = \frac{a}{2} \quad b^* = \frac{b}{2}\)  
Origin at 0,0,z

Along [1,0,0] c2mm1'  
\(a^* = b \quad b^* = c\)  
Origin at x,0,3/8

Along [1,1,0] c2m'm'  
\(a^* = \frac{(-a + b)}{2} \quad b^* = \frac{c}{2}\)  
Origin at x,x,0

\[
\begin{array}{llll}
4 & b & \bar{4}2'm' & 0,0,1/2 \ [0,0,w] \\
4 & a & \bar{4}2'm' & 0,0,0 \ [0,0,w] \\
\end{array}
\]

\[
\begin{array}{llll}
& & 0,1/2,3/4 \ [0,0,\bar{w}] & \\
& & 0,1/2,1/4 \ [0,0,\bar{w}] & \\
\end{array}
\]
Origin at $\overline{4}m'2$ at 0,1/4,-1/8 from center (2/m')

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For (0,0,0) + set

(1) 1  
   (1) 0,0,0
(5) 2 (0,1/2,0) 0,y,1/8  
   (2) x,1/4,1/8  
   (2) x,1/4,1/8
(9) $\overline{1}$ 0,1/4,1/8  
   (10) b' (0,1/2,0) x,y,1/8  
   (10) b' (0,1/2,0) x,y,1/8
(13) m' x,0,z  
   (14) m' 0,y,z  
   (14) m' 0,y,z

(2) 0,0,z  
   (2) $z$,0,0  
   (2) 0,0,z
(6) x,1/4,1/8  
   (6) x,1/4,1/8
(10) b' (0,1/2,0) x,y,1/8  
   (10) b' (0,1/2,0) x,y,1/8
(13) m' x,0,z  
   (14) m' 0,y,z  
   (14) m' 0,y,z

(3) $4'$ (0,0,1/4) -1/4,1/4,z  
   (3) $4'$ (0,0,1/4) -1/4,1/4,z
   (4) $4'$ (0,0,1/4) 1/4,1/4,z  
   (4) $4'$ (0,0,1/4) 1/4,1/4,z
(7) 2 x,y,0  
   (7) 2 x,y,0
(8) 2 x,y,0  
   (8) 2 x,y,0
(11) $4'$ 0,0,0; 0,0,0  
   (11) $4'$ 0,0,0; 0,0,0
(12) $4'$ 0,0,0; 0,0,0  
   (12) $4'$ 0,0,0; 0,0,0

(15) $d'$ (-1/4,1/4,1/4) x+1/4,x,z  
   (15) $d'$ (-1/4,1/4,1/4) x+1/4,x,z
(16) $d'(1/4,1/4,1/4) x-1/4,x,z  
   (16) $d'(1/4,1/4,1/4) x-1/4,x,z
(17) $m$ 0,1/2,1/4')  
   (17) $m$ 0,1/2,1/4')
(18) $m$ 0,1/2,1/4')  
   (18) $m$ 0,1/2,1/4')

141.9.1221 - 1 - 2613
For (1/2,1/2,1/2) + set

<table>
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<tr>
<th>Position</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>(1) t (1/2,1/2,1/2)</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>(2) 2 (0,0,1/2)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(3) 4*(0,0,3/4)</td>
<td>y,x,z [u,v,w]</td>
</tr>
<tr>
<td>(4) 4*(0,0,3/4)</td>
<td>y,1/2,x,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>(5) 2 1/4,y,3/8</td>
<td>y,x+1/2,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>(6) 2 (1/2,0,0)</td>
<td>x,y+1/2,z+1/4 [u,v,w]</td>
</tr>
<tr>
<td>(7) 2 (1/2,1/2,0)</td>
<td>x,x+1/4,1/2,3/8 [0,u,0]</td>
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<tr>
<td>(8) 2 x,x+1/2,1/4</td>
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<tr>
<td>(9) T</td>
<td>x,y,3/8</td>
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<tr>
<td>(10) a' (1/2,0,0)</td>
<td>x,y,1/2,z+1/4 [v,0,w]</td>
</tr>
<tr>
<td>(11) 4*</td>
<td>x,y,1/2,z</td>
</tr>
<tr>
<td>(12) 4*</td>
<td>0,1/2,z</td>
</tr>
<tr>
<td>(13) n' (1/2,0,1/2)</td>
<td>x,1/4,z</td>
</tr>
<tr>
<td>(14) n' (0,1/2,1/2)</td>
<td>1/4,y,z</td>
</tr>
<tr>
<td>(15) d' (1/4,-1/4,3/4)</td>
<td>x+1/4, x,z</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

**Positions**

Multiplicity,
Wyckoff letter,
Site Symmetry letter.

**Coordinates**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Generators</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>16 h .m'</td>
<td>(0,y,z [0,v,w]</td>
</tr>
<tr>
<td>16 g .2</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>16 f .2</td>
<td>x,1/4,1/8 [u,0,0]</td>
</tr>
<tr>
<td>8 e 2m'm'</td>
<td>0,0,0 [0,0,w]</td>
</tr>
<tr>
<td>8 d .2m'</td>
<td>0,1/4,5/8 [0,0,0]</td>
</tr>
<tr>
<td>8 c .2m'</td>
<td>0,1/4,1/8 [0,0,0]</td>
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</table>
Continued

4 b  4'2m' 0,0,1/2 [0,0,0]  0,1/2,3/4 [0,0,0]
4 a  4'2m' 0,0,0 [0,0,0]  0,1/2,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4m'm'
\[ \mathbf{a}' = \frac{\mathbf{a}}{2}, \quad \mathbf{b}' = \frac{\mathbf{b}}{2} \]
Origin at 0,0,z

Along [1,0,0]  c2m'm'
\[ \mathbf{a}' = \mathbf{b}, \quad \mathbf{b}' = \mathbf{c} \]
Origin at x,0,3/8

Along [1,1,0]  c2mm'
\[ \mathbf{a}' = \frac{-\mathbf{c}}{2}, \quad \mathbf{b}' = \frac{(-\mathbf{a} + \mathbf{b})}{2} \]
Origin at x,x,0
I4₁/acd

4/mmm

Tetragonal

I4₁/a2/c2/d

Origin at $\bar{4}c2$, at 0,1/4,-1/8 from $\bar{1}$

Asymmetric unit

$0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(5) 2 (0,1/2,0) 0,y,3/8
(2, 0,1/2,3/4)

(9) $\bar{1}$ 0,1/4,1/8
(1) 0,1/2,1/4)

(13) c (0,0,1/2) x,0,z
(m,0,0,1/2)

(14) c (0,0,1/2) x,0,y
(m,0,0,1/2)

(15) d (-1/4,1/4,3/4) x+1/4,y,z
(m,0,1/2,3/4)

(6) 2 x,1/4,3/8
(2, 0,1/2,3/4)

(10) b (0,1/2,0) x,y,1/8
(m,0,1/2,1/4)

(11) $\bar{4}^+$ 0,0,z; 0,0,0
(4,0,0,0)

(12) $\bar{4}^+$ 0,0,z; 0,0,0
(4,0,0,0)

(16) d (1/4,1/4,3/4) x-1/4,y,z
(m,0,1/2,3/4)
For (1/2, 1/2, 1/2) + set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
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<td>(2) 2 (0, 0, 1/2)</td>
<td>1/4, 1/4, z</td>
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<tr>
<td>(3) 4* (0, 0, 3/4)</td>
<td>1/4, 1/4, z</td>
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<tr>
<td>(4) 4* (0, 0, 3/4)</td>
<td>1/4, 1/4, z</td>
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<tr>
<td>(5) 2 1/4, y, 1/8</td>
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</tr>
<tr>
<td>(6) 2 (1/2, 0, 0)</td>
<td>x, 0, 1/8</td>
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<td>(7) 2 (1/2, 1/2, 0)</td>
<td>x, x, 0</td>
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<td>(8) 2 x, x + 1/2, 0</td>
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<td>(9) 1/4, y, 1/8</td>
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<td>(10) a (1/2, 0, 0)</td>
<td>x, y, 3/8</td>
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<td>(11) 1/4, y, 1/8</td>
<td>z, 1/2, 0, 1/4</td>
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<td>1/4, y, z</td>
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<td>(15) d (1/4, 1/4, 1/4)</td>
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<td>(16) d (1/4, 1/4, 1/4)</td>
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Generators selected

(1); t(1, 0, 0); t(0, 1, 0); t(0, 0, 1); t(1/2, 1/2, 1/2); (2); (3); (5); (9).

Positions

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<th>Site Symmetry</th>
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<td>x, y + 1/2, z + 3/4 [u, v, w]</td>
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<td>(7)</td>
<td>y, x + 1/2 [v, u, w]</td>
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<td>(9)</td>
<td>x, y + 1/2, z + 1/4 [u, v, w]</td>
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<td>(11)</td>
<td>y, x + 1/2 [v, u, w]</td>
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<tr>
<td>(13)</td>
<td>x, y, z + 1/2 [u, v, w]</td>
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</tr>
<tr>
<td>(15)</td>
<td>x, x + 1/2, z + 3/4 [u, v, w]</td>
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<td>x, x + 1/2, 1/2 [u, u, 0]</td>
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<td>(4)</td>
<td>y, x + 1/2, 1/2 [v, u, w]</td>
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<td>(5)</td>
<td>x, x + 1/2, 0 [u, u, 0]</td>
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<td>x, x, 3/4 [u, u, 0]</td>
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<td>x, x + 1/2, 0 [u, u, 0]</td>
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<td>y, x, z [v, u, w]</td>
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<td>x, y + 1/2, z + 1/4 [v, u, w]</td>
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<td>y, x, z [v, u, w]</td>
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<td>y, x, z [v, u, w]</td>
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<td>x, y, z + 1/2 [u, v, w]</td>
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<td>(14)</td>
<td>x, y, z + 1/2 [u, v, w]</td>
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<td>(15)</td>
<td>y, x + 1/2, z + 3/4 [v, u, w]</td>
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<td>(4)</td>
<td>3/4, y, 1/8 [0, v, 0]</td>
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<td>(6)</td>
<td>y, 1/4, 3/8 [v, 0, 0]</td>
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<td>(3)</td>
<td>0, 0, z + 1/2 [0, 0, w]</td>
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<td>(4)</td>
<td>0, 0, z + 1/2 [0, 0, w]</td>
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<table>
<thead>
<tr>
<th>16</th>
<th>c .1</th>
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<td>0, 1/4, 1/8 [u, v, w]</td>
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<td>0, 1/4, 1/8 [u, v, w]</td>
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<td>0, 1/4, 1/8 [u, v, w]</td>
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<tr>
<td>(4)</td>
<td>0, 1/2, 1/2 [0, 0, 0]</td>
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</table>
Symmetry of Special Projections

Along [0,0,1]  \( p_{\|} \) 4\( m'm' \)
\( a^* = a/2 \)  \( b^* = b/2 \)
Origin at 1/4,1/4,z

Along [1,0,0]  \( p_{\|} \) 2mm
\( a^* = b/2 \)  \( b^* = c/2 \)
Origin at x,0,1/8

Along [1,1,0]  \( c_{\|} \) 2\( m'm' \)
\( a^* = (-a + b)/2 \)  \( b^* = c/2 \)
Origin at x,x,0
I4₁/acd₁'
142.2.1223

4/mmm₁'
Tetragonal

I4₁/a2/c2/d₁'
142.2.1223

Origin at $\bar{4}c2₁$ at 0,1/4,-1/8 from $\bar{1} 1'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For (0,0,0) + set

(1) 1
(1' | 0,0,0)

(5) 2 (0,1/2,0) 0,y,3/8
(2, | 0,1/2,3/4)

(9) $\bar{1}$ 0,1/4,1/8
(1' | 0,1/2,1/4)

(13) c (0,0,1/2) x,0,z
(m, | 0,0,1/2)

(2) 2 0,0,z
(2, | 0,0,0)

(6) 2 x,1/4,3/8
(2, | 0,1/2,3/4)

(10) b (0,1/2,0) x,y,1/8
(m, | 0,1/2,1/4)

(3) $4^+$ (0,0,1/4) -1/4,1/4,z
(4,z | 0,1/2,1/4)

(7) 2 x,x,1/4
(2, | 0,0,1/2)

(11) $\bar{4}^+$ 0,0,z; 0,0,0
(4,z | 0,0,0)

(8) 2 x,x,1/4
(2, | 0,0,1/2)

(12) $\bar{4}^+$ 0,0,z; 0,0,0
(4,z | 0,0,0)

(14) c (0,0,1/2) 0,y,z
(m, | 0,0,1/2)

(15) d (-1/4,1/4,3/4) x+1/4,x,z
(m, | 0,1/2,3/4)

(16) d (1/4,1/4,3/4) x-1/4,x,z
(m, | 0,1/2,3/4)
Continued

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) (2) 2 (0,0,1/2) 1/4,1/4,z (3) 4 t (0,0,3/4) 1/4,1/4,z (4) 4' (0,0,3/4) 1/4,-1/4,z
(1 1/2,1/2,1/2) (2z z 1/2,1/2,1/2) (4z 1/2,0,3/4) (4z 1/2,0,3/4)

(5) 2 1/4,y,1/8 (6) 2 (1/2,0,0) x,0,1/8 (7) 2 (1/2,1/2,0) x,x,0
(2z 1/2,0,1/4) (2z 1/2,0,1/4) (2y 1/2,1/2,0) (2y 1/2,1/2,0)

(9) 1/4,0,3/8 (10) a (1/2,0,0) x,y,3/8 (11) 4 * (1/2,0,2,0)z; 1/2,0,1/4
(1/2,0,3/4) (mz 1/2,0,3/4) (4z 1/2,1/2,1/2) (4z 1/2,1/2,1/2)

(13) a (1/2,0,0) x,1/4,z (14) b (0,1/2,0) 1/4,y,z
(mz 1/2,1/2,0) (mx 1/2,1/2,0) (my 1/2,1/2,0)

For (0,0,0)' + set

(1) 1' (2) 2' 0,0,z (3) 4' (0,0,1/4) -1/4,1/4,z (4) 4' (0,0,1/4) 1/4,1/4,z
(1 0,0,0)' (2z 0,0,0)' (4z 0,1/2,1/4)' (4z 0,1/2,1/4)'

(5) 2' (0,1/2,0) 0,0,1/8 (6) 2' x,1/4,3/8 (7) 2' x,x,1/4
(2z 0,1/2,3/4)' (2z 0,1/2,3/4)' (2y 0,0,1/2)'

(9) 1/4,1/8 (10) b' (0,1/2,0) x,y,1/8 (11) 4 - (0,0,0,0)z; 0,0,0
(1/2,1/4) (mz 1/2,1/2,1/4)' (4z 0,0,0)'

(13) c' (0,0,1/2) x,0,z (14) c' (0,0,1/2) 0,y,z
(mz 0,0,1/2) (mx 0,0,1/2) (my 0,0,1/2)

For (1/2,1/2,1/2)' + set

(1) t' (1/2,1/2,1/2) (2) 2' (0,0,1/2) 1/4,1/4,z (3) 4' (0,0,3/4) 1/4,1/4,z (4) 4' (0,0,3/4) 1/4,-1/4,z
(1 1/2,1/2,1/2)' (2z 1/2,1/2,1/2)' (4z 1/2,0,3/4)' (4z 1/2,0,3/4)'

(5) 2' 1/4,y,1/8 (6) 2' (1/2,0,0) x,0,1/8 (7) 2' (1/2,1/2,0) x,x,0
(2z 1/2,0,1/4)' (2z 1/2,0,1/4)' (2y 1/2,1/2,0)'

(9) 1/4,0,3/8 (10) a' (1/2,0,0) x,y,3/8 (11) 4' * (1/2,0,2,0)z; 1/2,0,1/4
(1/2,0,3/4)' (mz 1/2,0,3/4)' (4z 1/2,1/2,1/2)' (4z 1/2,1/2,1/2)'

(13) a' (1/2,0,0) x,1/4,z (14) b' (0,1/2,0) 1/4,y,z
(mz 1/2,1/2,0)' (mx 1/2,1/2,0)' (my 1/2,1/2,0)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9); 1'.

Coordinates

(0,0,0) + (1/2,1/2,1/2) +
(0,0,0)' + (1/2,1/2,1/2)'

142.2.1223 - 2 - 2620
32 g 11' (1) x,y,z [0,0,0]  (2) x, y,z [0,0,0]
(3) y,x+1/2,z+1/4 [0,0,0]  (4) y,x+1/2,z+1/4 [0,0,0]
(5) x,y+1/2,z+3/4 [0,0,0]  (6) x,y+1/2,z+3/4 [0,0,0]
(7) y,x,z+1/2 [0,0,0]  (8) y,x,z+1/2 [0,0,0]
(9) x,y+1/2,z+1/4 [0,0,0]  (10) x,y+1/2,z+1/4 [0,0,0]
(11) y,x,z [0,0,0]  (12) y,x,z [0,0,0]
(13) x,y,z+1/2 [0,0,0]  (14) x,y,z+1/2 [0,0,0]
(15) y,x,z+1/2,z+3/4 [0,0,0]  (16) y,x,z+1/2,z+3/4 [0,0,0]
16 f .21' x,x,1/4 [0,0,0] x,x,1/4 [0,0,0] x,x+1/2,1/2 [0,0,0] x,x+1/2,1/2 [0,0,0]
x,x+1/2,0 [0,0,0] x,x+1/2,0 [0,0,0] x,x,3/4 [0,0,0] x,x,3/4 [0,0,0]
16 e .2.1' 1/4,y,1/8 [0,0,0] 3/4,y,1/8 [0,0,0] y,3/4,3/8 [0,0,0] y,1/4,3/8 [0,0,0]
3/4,y+1/2,1/8 [0,0,0] 1/4,y+1/2,1/8 [0,0,0] y,3/4,7/8 [0,0,0] y,1/4,7/8 [0,0,0]
16 d 2..1' 0,0,z [0,0,0] 0,1/2,z+1/4 [0,0,0] 0,1/2,z+3/4 [0,0,0] 0,0,z+1/2 [0,0,0]
0,1/2,z+1/4 [0,0,0] 0,0,z [0,0,0] 0,0,z+1/2 [0,0,0] 0,1/2,z+3/4 [0,0,0]
16 c 11' 0,1/4,1/8 [0,0,0] 0,3/4,1/8 [0,0,0] 3/4,1/2,3/8 [0,0,0] 1/4,1/2,3/8 [0,0,0]
0,3/4,5/8 [0,0,0] 0,1/4,5/8 [0,0,0] 1/4,0,3/8 [0,0,0] 3/4,0,3/8 [0,0,0]
8 b 2.221' 0,0,1/4 [0,0,0] 0,1/2,1/2 [0,0,0] 0,1/2,0 [0,0,0] 0,0,3/4 [0,0,0]
4 a 4..1' 0,0,0 [0,0,0] 0,1/2,1/4 [0,0,0] 0,1/2,3/4 [0,0,0] 0,0,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  
\[ a^* = a/2 \quad b^* = b/2 \]  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\[ a^* = b/2 \quad b^* = c/2 \]  
Origin at x,0,1/8

Along [1,1,0] c2mm1'  
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]  
Origin at x,x,0
Tetragonal

I4₁/a'cd

142.3.1224

4/m'mm

I4₁/a'2'/c2'/d

Origin

at \( \bar{4} 'c2' \) at 0,1/4,-1/8 from \( \bar{1} ' \)

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/8 \]

Symmetry Operations

For \( (0,0,0) + \text{ set} \)

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2_z \vert 0,0,0) \\
(3) & \quad 4^+ \quad (0,0,1/4) \quad -1/4,1/4,z \\
& \quad (4_z \vert 0,1/2,1/4) \\
(4) & \quad 4^- \quad (0,0,1/4) \quad 1/4,1/4,z \\
& \quad (4_z' \vert 0,1/2,1/4) \\
(5) & \quad 2' \quad (0,1/2,0) \quad 0,y,3/8 \\
& \quad (2_z \vert 0,1/2,3/4) \\
(6) & \quad 2' \quad x,1/4,3/8 \\
& \quad (2_z \vert 0,1/2,3/4) \\
(7) & \quad 2' \quad x,x,1/4 \\
& \quad (2_{xy} \vert 0,0,1/2) \\
(8) & \quad 2' \quad x,x,1/4 \\
& \quad (2_{xy} \vert 0,0,1/2) \\
(9) & \quad \bar{1}' \quad 0,1/4,1/8 \\
& \quad (1 \vert 0,1/2,1/4) \\
(10) & \quad b' \quad (0,1/2,0) \quad x,y,1/8 \\
& \quad (m_z \vert 0,1/2,1/4) \\
(11) & \quad \bar{4}^+ \quad x,0,z; \quad 0,0,0 \\
& \quad (4_z \vert 0,0,0) \\
(12) & \quad \bar{4}^- \quad x,0,z; \quad 0,0,0 \\
& \quad (4_{z'} \vert 0,0,0) \\
(13) & \quad c \quad (0,0,1/2) \quad x,0,z \\
& \quad (m_{xy} \vert 0,0,1/2) \\
(14) & \quad c \quad (0,0,1/2) \quad 0,y,z \\
& \quad (m_{xy} \vert 0,0,1/2) \\
(15) & \quad d \quad (-1/4,1/4,3/4) \quad x+1/4,\bar{x},z \\
& \quad (m_{x} \vert 0,1/2,3/4) \\
(16) & \quad d \quad (1/4,1/4,3/4) \quad x-1/4,\bar{x},z \\
& \quad (m_{x} \vert 0,1/2,3/4)
\end{align*}
Continued

For (1/2,1/2,1/2) + set

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Generator(s)</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
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<td>(3) y + x + 1/2, z + 1/4 [v,u,w]</td>
<td>(4) y + x + 1/2, z + 1/4 [v,u,w]</td>
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<td>(5) x + y + 1/2, z + 3/4 [u,v,w]</td>
<td>(6) x + y + 1/2, z + 3/4 [u,v,w]</td>
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<tr>
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<td>(7) y + x + 1/2 [v,u,w]</td>
<td>(8) y + x + 1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x + y + 1/2, z + 1/4 [v,u,w]</td>
<td>(10) x + y + 1/2, z + 1/4 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x + y, z [v,u,w]</td>
<td>(12) x + y, z [v,u,w]</td>
</tr>
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<td>(13) x + y, z + 1/2 [v,u,w]</td>
<td>(14) x + y, z + 1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(15) x + y + 1/2, z + 3/4 [v,u,w]</td>
<td>(16) x + y + 1/2, z + 3/4 [v,u,w]</td>
</tr>
</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

Wyckoff letter, Site Symmetry.

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<th>Coordinates</th>
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<td>16 f .2'</td>
<td>x + 1/4 [u,u,w]</td>
<td>x + 1/4 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x + 1/2 [u,u,w]</td>
<td>x + 1/2 [u,u,w]</td>
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<tr>
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<td>x + 3/4 [u,u,w]</td>
<td>x + 3/4 [u,u,w]</td>
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<td>0,1/2,1/2 [0,0,w]</td>
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<tr>
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<td>0,0,3/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>
Continued 142.3.1224 I4, /a'cd

| 4 | a | \(4'\) | 0,0,0 [0,0,0] | 0,1/2,1/4 [0,0,0] | 0,1/2,3/4 [0,0,0] | 0,0,1/2 [0,0,0] |

### Symmetry of Special Projections

- **Along [0,0,1] p4mm**
  \[a^* = a/2 \quad b^* = b/2\]
  Origin at 0,0,z

- **Along [1,0,0] p2mm**
  \[a^* = b/2 \quad b^* = c/2\]
  Origin at x,1/4,3/8

- **Along [1,1,0] c2'mm'**
  \[a^* = -c/2 \quad b^* = (-a + b)/2\]
  Origin at x,x,0
Origin at $\bar{4}$c$'$2, at 0,1/4,-1/8 from 1

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/8$

Symmetry Operations

For (0,0,0) + set

(1) $1$
   (1 0 0)

(5) 2' (0,1/2,0) 0,y,3/8
    (2, 0,1/2,3/4)

(9) $\bar{1}$ 0,1/4,1/8
    (1 0,1/2,1/4)

(13) c' (0,0,1/2) x,0,z
     (m, 0,0,1/2)

(2) 2 0,0,z
    (2z, 0,0,0)

(6) 2' x,1/4,3/8
    (2z, 0,1/2,3/4)

(10) b (0,1/2,0) x,y,1/8
     (m, 0,1/2,1/4)

(14) c' (0,0,1/2) 0,y,z
     (m, 0,0,1/2)

(3) 4' (0,0,1/4) -1/4,1/4,z
    (4z 0,1/2,1/4)

(7) 2 x,x,1/4
    (2y, 0,0,1/2)

(11) $\bar{4}$' 0,0,z
     (4z 0,0,0)

(15) d (-1/4,1/4,3/4) x+1/4,x,z
     (m 0,1/2,3/4)

(4) 4' (0,0,1/4) 1/4,1/4,z
    (4z 1/2,1/4)

(8) 2 x,x,1/4
    (2y, 0,0,1/2)

(12) $\bar{4}$' 0,0,z
     (4z 0,0,0)

(16) d (1/4,1/4,3/4) x-1/4,x,z
     (m 0,1/2,3/4)
Continued

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(2) 2 (0,0,1/2) 1/4,1/4,z
(3) 4* (0,0,3/4) 1/4,1/4,z
(4) 4* (0,0,3/4) 1/4,-1/4,z

(5) 2' 1/4,y,1/8
(6) 2' (1/2,0,0) x,0,1/8
(7) 2 (1/2,0,1/2) x,x,0
(8) 2 (0,0,3/4) 1/4,-1/4,z

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

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<td>(9) x,y+1/2,z+1/4 [u,v,w]</td>
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<td>(15) y,x+1/2,z+3/4 [v,u,w]</td>
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<tr>
<td>3/4,y,1/8 [u,0,w]</td>
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</tr>
<tr>
<td>3/4,y,1/8 [u,0,w]</td>
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<td>3/4,y,1/8 [u,0,w]</td>
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<td>3/4,y,1/8 [u,0,w]</td>
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<table>
<thead>
<tr>
<th>16</th>
<th>d 2..</th>
</tr>
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<tbody>
<tr>
<td>0,0,z [0,0,w]</td>
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</tr>
<tr>
<td>0,1/2,z+1/4 [0,0,w]</td>
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<tr>
<td>0,1/2,z+1/4 [0,0,w]</td>
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<tr>
<td>0,1/2,z+1/4 [0,0,w]</td>
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<tr>
<td>0,1/2,z+1/4 [0,0,w]</td>
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<table>
<thead>
<tr>
<th>16</th>
<th>c .1</th>
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</thead>
<tbody>
<tr>
<td>0,1,4,1/8 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>0,3/4,1/8 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>0,3/4,5/8 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>0,1,4,1/8 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td>0,3/4,3/8 [v,u,w]</td>
<td></td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>8</th>
<th>b 2.22</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>0,1,2/2 [0,0,0]</td>
<td></td>
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<tr>
<td>0,1,2/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>0,0,3/4 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] \( p^* \) 4m'm'
\( a^* = a/2 \quad b^* = b/2 \)
Origin at 0,0,z

Along [1,0,0] \( p^* \) 2mm
\( a^* = b/2 \quad b^* = c/2 \)
Origin at x,1/4,1/8

Along [1,1,0] \( c^* \) 2m'm'
\( a^* = (-a + b)/2 \quad b^* = c/2 \)
Origin at x,x,0
I4₁'/ac₁'d

142.5.1226

I4₁'/a₂/c₂'d

Tetragonal

4'/mmm'

Origin at \( 4'c₂', \) at 0,1/4,-1/8 from \( 1' \)

Asymmetric unit: \( 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8 \)

Symmetry Operations

For \((0,0,0) + \) set

(1) \( 1 \)

(1|0,0,0)

(5) \( 2 \) \( (0,1/2,0) \) \( 0,\text{y},3/8 \)

(2,1/2,3/4)

(9) \( \bar{1} \) \( 0,1/4,1/8 \)

(1|0,1/2,1/4)

(13) \( c \) \( (0,0,1/2) \) \( x,0,z \)

(m,1/2,0)

(2) \( 2 \) \( 0,0,z \)

(2Z|0,0,0)

(6) \( 2 \) \( x,1/4,3/8 \)

(2Z|0,1/2,3/4)

(10) \( b \) \( (0,1/2,0) \) \( x,y,1/8 \)

(mZ|0,1/2,1/4)

(2) \( 2' \)

(2Z|0,1/2,3/4)

(14) \( c \) \( (0,0,1/2) \) \( 0,\text{y},z \)

(m,0,0,1/2)

(15) \( d' \) \((1/4,1/4,3/4)\) \( x+1/4,\text{x},z \)

(4mZ|0,1/2,3/4)

(11) \( 4^+ \) \((0,0,1/4)\) \(-1/4,1/4,z \)

(4Z|0,1/2,1/4)

(12) \( 4^+ \) \((0,0,1/4)\) \(1/4,1/4,z \)

(4Z^-1|0,1/2,1/4)

(16) \( d' \) \((1/4,1/4,3/4)\) \( x-1/4,\text{x},z \)

(4mZ|0,1/2,3/4)

(17) \( 4^+ \) \((0,0,1/4)\) \(1/4,1/4,z \)

(4Z^-1|0,0,0)
For \((1/2, 1/2, 1/2) + \) set

\[
\begin{align*}
(1) & \ t(1/2, 1/2, 1/2) \\
(2) & \ 2(0, 0, 1/2) \\
(3) & \ 4' (0, 0, 3/4) \\
(4) & \ 4' (0, 0, 3/4) \\
& \ 4' (1/2, 2/0, 3/4) \\
& \ 4' (1/2, 2/0, 3/4) \\
(5) & \ 2(1/4, y, 1/8) \\
(6) & \ 2(1/2, 0, 0) \\
(7) & \ 2' (1/2, 1/2, 0) \\
(8) & \ 2' x, x + 1/2, 0 \\
(9) & \ 1/4, 0, 3/8 \\
(10) & \ a(1/2, 0, 0) \\
(11) & \ 4' (1/2, 0, 2/0, 1/4) \\
(12) & \ 4' (1/2, 0, 2/0, 1/4) \\
(13) & \ a(1/2, 0, 0) \\
(14) & \ b(0, 1/2, 0) \\
(15) & \ d'(1/4, -1/4, 1/4) \\
(16) & \ d'(1/4, 1/4, 1/4) \\
\end{align*}
\]

Generators selected \((1); t(1, 0, 0); t(0, 1, 0); t(0, 0, 1); t(1/2, 1/2, 1/2); (2); (3); (5); (9).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

\[
\begin{align*}
(0, 0, 0) + & \ (1/2, 1/2, 1/2) + \\
32 & \ g \ 1 \ \\
(1) & \ x, y, z [u, v, w] \\
(2) & \ y, x, z [u, v, w] \\
(3) & \ y, x, +1/2, z +1/4 [v, u, w] \\
(4) & \ y, x, +1/2, z +1/4 [v, u, w] \\
(5) & \ x, y, +1/2, z +3/4 [u, v, w] \\
(6) & \ x, y, +1/2, z +3/4 [u, v, w] \\
(7) & \ y, x, +1/2 [v, u, w] \\
(8) & \ y, x, +1/2 [v, u, w] \\
(9) & \ x, y, z +1/2 [u, v, w] \\
(10) & \ y, x, z +1/2 [v, u, w] \\
(11) & \ y, x, z +1/2 [v, u, w] \\
(12) & \ x, y, z +1/2 [u, v, w] \\
(13) & \ x, y, z +1/2 [u, v, w] \\
(14) & \ x, y, z +1/2 [u, v, w] \\
(15) & \ x, y, z +1/2, z +3/4 [v, u, w] \\
(16) & \ x, y, z +1/2, z +3/4 [v, u, w] \\
\end{align*}
\]
Symmetry of Special Projections

Along [0,0,1] \( p_c \) 4mm
\[ a^* = \frac{a}{2}, \quad b^* = \frac{b}{2} \]
Origin at 0,0,z

Along [1,0,0] \( p_a \) 2mm
\[ a^* = \frac{b}{2}, \quad b^* = \frac{c}{2} \]
Origin at x,1/4,1/8

Along [1,1,0] \( c \) 2mm'
\[ a^* = -\frac{c}{2}, \quad b^* = \frac{-a + b}{2} \]
Origin at x,x,0
Origin at $\bar{4}c'2'$ at \(0,1/4,-1/8\) from $\bar{1}'$.

Asymmetric unit
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8\]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\)
   \(1\) \(0,0,0\)

2. \(2\)
   
   \(0,0,z\)
   \(\left(\bar{2}_z|0,0,0\right)\)

3. \(4'\)
   
   \((0,0,1/4)\)
   \(-1/4,1/4,z\)
   \(\left(4_z|0,1/2,1/4\right)'\)

4. \(4'\)
   
   \((0,0,1/4)\)
   \(1/4,1/4,z\)
   \(\left(4_z^{-1}|0,1/2,1/4\right)'\)

5. \(2\)
   
   \((0,1/2,0)\)
   \(0,y,3/8\)
   \(\left(2_y|0,1/2,3/4\right)\)

6. \(2\)
   
   \((0,1/2,0)\)
   \(x,1/4,3/8\)
   \(\left(2_x|0,1/2,3/4\right)\)

7. \(2'\)
   
   \((x,x,1/4)\)
   \((2_{xy}|0,0,1/2)'\)

8. \(2'\)
   
   \((x,x,1/4)\)
   \((2_{xy}|0,0,1/2)'\)

9. \(\bar{1}'\)
   
   \((1/2,0,1/4)\)
   \(0,1/4,1/8\)
   \(\left(\bar{1}_x|0,1/2,1/4\right)'\)

10. \(2'\)
    
    \((0,1/2,0)\)
    \(x,y,1/8\)
    \(\left(m_y|0,1/2,1/4\right)\)

11. \(4'\)
    
    \((0,0,0)\)
    \(0,0,0\)
    \(\left(4_z|0,0,0\right)'\)

12. \(4'\)
    
    \((0,0,0)\)
    \(0,0,0\)
    \(\left(4_z^{-1}|0,0,0\right)'\)

13. \(c'\)
    
    \((0,0,1/2)\)
    \(x,0,z\)
    \(\left(m_x|0,0,1/2\right)'\)

14. \(c'\)
    
    \((0,0,1/2)\)
    \(0,y,z\)
    \(\left(m_x|0,0,1/2\right)'\)

15. \(d\)
    
    \((-1/4,1/4,3/4)\)
    \(x+1/4,x,z\)
    \(\left(m_{xy}|0,1/2,3/4\right)\)

16. \(d\)
    
    \((1/4,1/4,3/4)\)
    \(x-1/4,x,z\)
    \(\left(m_{xy}|0,1/2,3/4\right)\)

For \((1/2,1/2,1/2) + \) set

1. \(t\)
   
   \((1/2,1/2,1/2)\)
   \((1/2,1/2,1/2)\)

2. \(2\)
   
   \((0,0,1/2)\)
   \(1/4,1/4,z\)
   \(\left(2_z|1/2,1/2,1/2\right)\)

3. \(4'\)
   
   \((0,0,3/4)\)
   \(1/4,1/4,z\)
   \(\left(4_z|1/2,0,3/4\right)'\)

4. \(4'\)
   
   \((0,0,3/4)\)
   \(1/4,-1/4,z\)
   \(\left(4_z^{-1}|1/2,0,3/4\right)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td>(2) x, y, z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) y, x+1/2, z+1/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) y, x+1/2, z+1/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) x, y+1/2, z+3/4 [u,v,w]</td>
<td></td>
</tr>
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<td>(6) x, y+1/2, z+3/4 [u,v,w]</td>
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</tr>
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<td></td>
<td>(7) y, x, z+1/2 [v,u,w]</td>
<td></td>
</tr>
<tr>
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<td>(8) y, x, z+1/2 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(9) x, y+1/2, z+1/4 [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(10) x, y+1/2, z+1/4 [u,v,w]</td>
<td></td>
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<tr>
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<td>(11) x, y, z [v,u,w]</td>
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<tr>
<td></td>
<td>(12) x, y, z [v,u,w]</td>
<td></td>
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<tr>
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<td>(13) x, y, z+1/2 [v,u,w]</td>
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<tr>
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<td>(14) x, y, z+1/2 [v,u,w]</td>
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</tr>
<tr>
<td></td>
<td>(15) y, x+1/2, z+3/4 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(16) y, x+1/2, z+3/4 [v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

| 16 f 2'      | x, x+1/1 [u,u,w] |
|              | x, x, 1/1 [u,u,w] |
|              | x, x+1/2, 1/2 [u,u,w] |
|              | x, x, 1/1 [u,u,w] |

| 16 e .2       | 1/4, y, 1/8 [0,v,0] |
|              | 3/4, 1/8 [0,v,0] |
|              | 3/4, 1/8 [0,v,0] |

| 16 d 2.       | 0, 0, z [0,0,0] |
|              | 0, 1/2, z+1/4 [0,0,0] |
|              | 0, 1/2, z+1/4 [0,0,0] |

| 16 c 1'       | 0, 1/4, 1/8 [0,0,0] |
|              | 0, 3/4, 1/8 [0,0,0] |
|              | 0, 3/4, 1/8 [0,0,0] |

| 8 b 2.2'      | 0, 0, 1/4 [0,0,0] |
|              | 0, 1/2, 1/2 [0,0,0] |
|              | 0, 0, 1/2 [0,0,0] |

| 4 a 2'       | 0, 0, 0 [0,0,0] |
|              | 0, 1/2, 1/4 [0,0,0] |
|              | 0, 0, 1/2 [0,0,0] |

Continued
## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Orientation</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p4'm'm</td>
<td>a* = a/2, b* = b/2</td>
<td>0,0,z</td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p2m'm'</td>
<td>a* = b/2, b* = c/2</td>
<td>x,0,1/8</td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>c_p 2m'm'</td>
<td>a* = (-a + b)/2, b* = c/2</td>
<td>x,x,0</td>
</tr>
</tbody>
</table>
I41/ac'd'
142.7.1228

I41/ac'd'

Tetragonal

Origin at $\overrightarrow{c}2'$, at 0,1/4,-1/8 from $\overrightarrow{1}$

Asymmetric unit
$0 \leq x \leq 1/2; \ 0 \leq y \leq 1/2; \ 0 \leq z \leq 1/8$

Symmetry Operations

For (0,0,0) + set

1. $1$

2. $2\cdot 0,0,z$
   $(2_{z}\cdot 0,0,0)$

3. $4^+ (0,0,1/4) -1/4,1/4,z$
   $(4_{z}\cdot 0,1/2,1/4)$

4. $4^- (0,0,1/4) 1/4,1/4,z$
   $(4_{z}^{-1}\cdot 0,1/2,1/4)$

5. $2' (0,1/2,0) 0,y,3/8$
   $(2_{y}\cdot 0,1/2,3/4)'

6. $2' \cdot x,1/4,3/8$
   $(2_{x}\cdot 0,1/2,3/4)'$

7. $2' \cdot x,x,1/4$
   $(2_{y}\cdot 0,0,1/2)'$

8. $2' \cdot x,x,1/4$
   $(2_{y}\cdot 0,0,1/2)'$

9. $\overrightarrow{1} 0,1/4,1/8$
   $(\overrightarrow{1}\cdot 0,1/2,1/4)$

10. $b (0,1/2,0) \cdot x,y,1/8$
    $(m_{x}\cdot 0,1/2,1/4)$

11. $4^+ 0,0,z; 0,0,0$
    $(4_{x}\cdot 0,0,0)$

12. $4^- 0,0,z; 0,0,0$
    $(4_{x}^{-1}\cdot 0,0,0)$

13. $c' (0,0,1/2) \cdot x,0,z$
    $(m_{x}\cdot 0,0,1/2)'$

14. $c' (0,0,1/2) \cdot 0,y,z$
    $(m_{x}\cdot 0,0,1/2)'$

15. $d' (-1/4,1/4,3/4) \cdot x+1/4,x,z$
    $(m_{x}\cdot 0,1/2,3/4)'$

16. $d' (1/4,1/4,3/4) \cdot x-1/4,x,z$
    $(m_{x}\cdot 0,1/2,3/4)'$
Continued

(1) t (1/2,1/2,1/2) + set
(1) 1/4,1/4,1/4
(2) 1/2,1/2,1/2
(3) 1/2,1/2,1/2
(4) 1/2,1/2,1/2

For (1/2,1/2,1/2) + set

(1) 1/2,1/2,1/2
(2) 1/2,1/2,1/2
(3) 1/2,1/2,1/2
(4) 1/2,1/2,1/2

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
</table>

| (0,0,0) + (1/2,1/2,1/2) + |
|----------------|----------------|---------------|

32 g 1

(1) x,y,z [u,v,w] (2) x,y,z [u,v,w]
(3) y,x+1/2,z+1/4 [v,u,w] (4) y,x+1/2,z+1/4 [v,u,w]
(5) x,y+1/2,z+3/4 [u,v,w] (6) x,y+1/2,z+3/4 [u,v,w]
(7) y,x,z+1/2 [v,u,w] (8) y,x,z+1/2 [v,u,w]
(9) x,y+1/2,z+1/4 [u,v,w] (10) x,y+1/2,z+1/4 [u,v,w]
(11) y,x,z [v,u,w] (12) y,x,z [v,u,w]
(13) x,y,z+1/2 [u,v,w] (14) x,y,z+1/2 [u,v,w]
(15) x,y+1/2,z+3/4 [v,u,w] (16) x,y+1/2,z+3/4 [v,u,w]

16 f .2’

x,x,1/4 [u,u,w] x,x+1/2,z+1/2 [u,u,w] x,x+1/2,z+1/2 [u,u,w] x,x+1/2,z+1/2 [u,u,w]

16 e .2’

1/4,y,1/8 [u,0,w] 3/4,y,1/8 [u,0,w] y,3/4,3/8 [0,u,w] y,1/4,3/8 [0,u,w]

16 d 2

0,0,z [0,0,w] 0,1/2,z+1/4 [0,0,w] 0,1/2,z+1/4 [0,0,w] 0,0,z+1/2 [0,0,w]

16 c T

0,1/4,1/8 [u,v,w] 0,3/4,1/8 [u,v,w] 3/4,1/2,3/8 [v,u,w] 1/4,1/2,3/8 [v,u,w]

8 b 2.2’

0,0,1/4 [0,0,w] 0,1/2,1/2 [0,0,w] 0,1/2,1/2 [0,0,w] 0,0,3/4 [0,0,w]
Symmetry of Special Projections

Along [0,0,1] \( p_4 \), 4\( m' \)n
\[ a^* = a/2 \quad b^* = b/2 \]
Origin at \( 1/4,1/4,z \)

Along [1,0,0] \( p2'm \)m'
\[ a^* = -c/2 \quad b^* = b/2 \]
Origin at \( x,0,1/8 \)

Along [1,1,0] \( c2'm' \)m'
\[ a^* = -c/2 \quad b^* = -(a + b)/2 \]
Origin at \( x,x,0 \)
I4₁'/a'cd' 142.8.1229

Tetragonal

4'/m'mm'
I4₁'/a'2'/c2/d'

Origin at 4c2, at 0,1/4,-1/8 from 1

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/8

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(5) 2' (0,1/2,0) 0,y,3/8
(2|0,1/2,3/4')

(9) 1' 0,1/4,1/8
(1|0,1/2,1/4')

(13) c (0,0,1/2) x,0,z
(m|0,0,1/2)

(2) 2 0,0,z
(2z|0,0,0)

(6) 2' x,1/4,3/8
(2z|0,1/2,3/4')

(10) b' (0,1/2,0) x,y,1/8
(m|0,1/2,1/4')

(3) 4+ (0,0,1/4) -1/4,1/4,z
(4z|0,1/2,1/4')

(7) 2 x,x,1/4
(2x|0,0,1/2)

(11) 4+ 0,0,z; 0,0,0
(4z|0,0,0)

(14) c (0,0,1/2) 0,y,z
(m|0,0,1/2)

(4) 4' (0,0,1/4) 1/4,1/4,z
(4z|0,1/2,1/4')

(8) 2 x,x,1/4
(2x|0,0,1/2)

(12) 4- 0,0,z; 0,0,0
(4z-1|0,0,0)

(15) d' (-1/4,1/4,3/4) x+1/4,x,z
(m|0,1/2,3/4')

(16) d' (1/4,1/4,3/4) x-1/4,x,z
(m|0,1/2,3/4')
For \((1/2,1/2,1/2) + \) set

\begin{align*}
(1) \ t & (1/2,1/2,1/2) \\
(2) \ 2 & (0,0,1/2) \ 1/4,1/4,z \\
(3) \ 4^* & (0,0,3/4) \ 1/4,1/4,z \\
(4) \ 4^* & (0,0,3/4) \ 1/4,1/4,z \\
(5) \ 2' & 1/4,y,1/8 \\
(6) \ 2' & (1/2,0,0) \ x,0,1/8 \\
(7) \ 2 & (1/2,1/2,0) \ x,x,0 \\
(8) \ 2 & x,x+1/2,0 \\
(9) \ a' & (1/2,0,0) \ x,y,z \\
(10) \ a' & (1/2,0,0) \ x,y+1/2,0 \\
(11) \ a' & (1/2,0,0) \ x,y+1/2,z+1/4 \\
(12) \ a' & (1/2,0,0) \ x,y+1/2,z+1/4 \\
(13) \ b & (0,1/2,0) \ 1/4,y,z \\
(14) \ b & (0,1/2,0) \ 1/4,y,z \\
(15) \ d' & (1/4,-1/4,1/4) \ x+1/4,x,z \\
(16) \ d' & (1/4,1/4,1/4) \ x+1/4,x,z \\
\end{align*}

Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9). \)

<table>
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<tr>
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<th>Coordinates</th>
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<tbody>
<tr>
<td>32</td>
<td>((0,0,0) + (1/2,1/2,1/2) + )</td>
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<tr>
<td>16</td>
<td>((0,0,0) + (1/2,1/2,1/2) + )</td>
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<td>16</td>
<td>((0,0,0) + (1/2,1/2,1/2) + )</td>
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<td>16</td>
<td>((0,0,0) + (1/2,1/2,1/2) + )</td>
</tr>
<tr>
<td>16</td>
<td>((0,0,0) + (1/2,1/2,1/2) + )</td>
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<tr>
<td>8</td>
<td>((0,0,0) + (1/2,1/2,1/2) + )</td>
</tr>
</tbody>
</table>

**Positions**

\begin{align*}
\text{Wyckoff letter} & \quad \text{Site Symmetry} \\
(1) \ x,y,z [u,v,w] & \quad (2) \ x,y,z [u,v,w] \\
(3) \ y,x+1/2,z+1/4 [v,u,w] & \quad (4) \ y,x+1/2,z+1/4 [v,u,w] \\
(5) \ x,y+1/2,z+3/4 [u,v,w] & \quad (6) \ x,y+1/2,z+3/4 [u,v,w] \\
(7) \ y,x,z+1/2 [v,u,w] & \quad (8) \ y,x,z+1/2 [v,u,w] \\
(9) \ x,y,z+1/2 [v,u,w] & \quad (10) \ x,y,z+1/2 [v,u,w] \\
(11) \ y,x,z [v,u,w] & \quad (12) \ y,x,z [v,u,w] \\
(13) \ x,y,z+1/2 [u,v,w] & \quad (14) \ x,y,z+1/2 [u,v,w] \\
(15) \ y,x+1/2,z+3/4 [v,u,w] & \quad (16) \ y,x+1/2,z+3/4 [v,u,w] \\
\end{align*}

**Groups**

\begin{align*}
\text{Continued} & \quad 142.8.1229 \\
\text{i4,'a'cd'} & \quad 142.8.1229 - 2 - 2638
\end{align*}
Symmetry of Special Projections

Along [0,0,1]  p4'mm'  
\[ \mathbf{a}^* = \mathbf{a}/2 \quad \mathbf{b}^* = \mathbf{b}/2 \]  
Origin at 0,0,z

Along [1,0,0]  p4 2mm  
\[ \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]  
Origin at x,1/4,1/8

Along [1,1,0]  c2m'm'  
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]  
Origin at x,x,0
Tetragonal

Origin at $\bar{4}c'2$, at $0,1/4,-1/8$ from $\bar{1}'$

Asymmetric unit $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/8$

Symmetry Operations

For $(0,0,0) +$ set

1. $1 \quad (1|0,0,0)$
2. $2 \quad 0,0,z \quad (2_z|0,0,0)$
3. $4^+ (0,0,1/4) \quad -1/4,1/4,z \quad (4_z|0,1/2,1/4)$
4. $4' (0,0,1/4) \quad 1/4,1/4,z \quad (4_z^{-1}|0,1/2,1/4)$
5. $2 \quad (0,1/2,0) \quad 0,y,3/8 \quad (2_x|0,1/2,3/4)$
6. $2 \quad x,1/4,3/8 \quad (2_x|0,1/2,3/4)$
7. $2 \quad x,x,1/4 \quad (2_{xy}|0,0,1/2)$
8. $2 \quad x,x,1/4 \quad (2_{xy}|0,0,1/2)$
9. $\bar{1}' \quad 0,1/4,1/8 \quad (\bar{1}|0,1/2,1/4)$
10. $b' (0,1/2,0) \quad x,y,1/8 \quad (m_x|0,1/2,1/4)$
11. $\bar{4}^+ \quad 0,0,z \quad 0,0,0 \quad (\bar{4}_x|0,0,0)$
12. $\bar{4}' \quad 0,0,z \quad 0,0,0 \quad (\bar{4}_x^{-1}|0,0,0)$
13. $c' (0,0,1/2) \quad x,0,z \quad (m_y|0,0,1/2)$
14. $c' (0,0,1/2) \quad 0,y,z \quad (m_y|0,0,1/2)$
15. $d^+ (-1/4,1/4,3/4) \quad x+1/4,y,z \quad (m_{xy}|0,1/2,3/4)$
16. $d' (1/4,1/4,3/4) \quad x-1/4,y,z \quad (m_{xy}|0,1/2,3/4)$
Continued

For (1/2,1/2,1/2) + set

<p>| | | | |</p>
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<tbody>
<tr>
<td>1</td>
<td>t (1/2,1/2,1/2)</td>
<td>(1) t (1/2,1/2,1/2)</td>
<td>(2) 2 (0,0,1/2)</td>
</tr>
<tr>
<td></td>
<td>(2z</td>
<td>1/2,1/2,1/2)</td>
<td>1/4,1/4,z</td>
</tr>
<tr>
<td></td>
<td>(4z</td>
<td>1/2,0,3/4)</td>
<td>1/4,1/4,z</td>
</tr>
<tr>
<td></td>
<td>(4z^2</td>
<td>1/2,0,3/4)</td>
<td>1/4,1/4,z</td>
</tr>
<tr>
<td>2</td>
<td>1/4,y,1/8</td>
<td>(6) 2 (1/2,0,0)</td>
<td>x,x,0</td>
</tr>
<tr>
<td></td>
<td>(2z</td>
<td>1/2,0,1/4)</td>
<td>1/4,1/4,z</td>
</tr>
</tbody>
</table>
| 3 | T 1/4,0,3/8 | (11) 4^+ · 1/2,0,z | 1/2,0,1/4 | (12) 4^+ · 1/2,1/2,1/2)
|   | (4z) | 1/2,2,3/4) | 1| z | 1/2,1/2,1/2) |
| 4 | a' (1/2,0,0) | (13) a' (1/2,0,0) | x,y,z | (14) b' (0,1/2,0) |
|   | (mz | 1/2,1/2,1/2) | 3/4,y,3/8 | (15) d' (1/2,1/2,1/2) |
|   | (mz | 1/2,1/2,1/2) | 3/4,y,3/8 | (mz | 1/2,0,1/4) |
| 5 | x,y+1/2,z+1/4 | (15) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (mx | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (mx | 1/2,0,1/4) | x,x,1/4 | (n | 1/2,0,1/4) |
| 6 | x,x+1/2,z+1/4 | (16) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (mx | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (mx | 1/2,0,1/4) | x,x,1/4 | (n | 1/2,0,1/4) |
| 7 | x+1/4,y,z+3/4 | (15) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (mx | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (mx | 1/2,0,1/4) | x,x,1/4 | (n | 1/2,0,1/4) |
| 8 | y,x,z+1/2 | (16) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
| 10 | x,y+1/2,z+1/4 | (16) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
| 11 | y,x,z+1/2 | (16) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
| 12 | y,x,z+1/2 | (16) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
| 13 | y,x,z+1/2 | (16) d' (1/2,1/2,1/2) | x+1/4,x,z | (16) d' (1/2,1/2,1/2) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |
|   | (y | 1/2,1/2,1/2) | x,x,1/4 | (n | 1/2,0,1/4) |

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (9).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>g</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>16</td>
<td>f</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>16</td>
<td>e</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>c</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>b</td>
<td></td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1]  p4m'm'
\[ a^* = \frac{a}{2} \quad b^* = \frac{b}{2} \]
Origin at 0,0,z

Along [1,0,0]  p2m'm'
\[ a^* = \frac{b}{2} \quad b^* = \frac{c}{2} \]
Origin at x,0,1/8

Along [1,1,0]  c2m'm'
\[ a^* = \frac{a + b}{2} \quad b^* = \frac{c}{2} \]
Origin at x,x,0
### Origin

On 3

### Asymmetric unit

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 2/3;</td>
<td>0 ≤ y ≤ 2/3;</td>
<td>0 ≤ z ≤ 1;</td>
</tr>
<tr>
<td>x ≤ (1+y)/2;</td>
<td>y ≤ min(1-x,(1+x)/2)</td>
<td></td>
</tr>
</tbody>
</table>

### Vertices

| 0,0,0 | 1/2,0,0 | 2/3,1/3,0 | 1/3,2/3,0 | 0,1/2,0 |
| 0,0,1 | 1/2,0,1 | 2/3,1/3,1 | 1/3,2/3,1 | 0,1/2,1 |

### Symmetry Operations

(1) 1
(1|0,0,0)

(2) 3* 0,0,z
(3z|0,0,0)

(3) 3 0,0,z
(3z⁻¹|0,0,0)
Continued 143.1.1231 P3

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(3) x +y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>1 c 3..</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>(2) y,x-y,z [v-u,v,w]</td>
</tr>
<tr>
<td>1 b 3..</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>1 a 3..</td>
<td>0,0,z [0,0,w]</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p3  
**a** = **a**  
**b** = **b**  
Origin at 0,0,z

Along [1,0,0] p1  
**a** = **c**  
**b** = (a + 2b)/2  
Origin at x,0,0

Along [2,1,0] p1  
**a** = **c**  
**b** = **b**/2  
Origin at x,x/2,0
Origin on $31'$

Asymmetric unit

$$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$$

Vertices

$$0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0$$

$$0,0,1 \quad 1/2,0,1 \quad 2/3,1/3,1 \quad 1/3,2/3,1 \quad 0,1/2,1$$

Symmetry Operations

For $1$ set

$$(1) \quad 1$$

$$(1') \quad 3'$$

$$(1' | 0,0,0)$$

$$(1' | 0,0,0)'$$

$$(1' | 0,0,0)'$$

$$(2) \quad 3'$$

$$(2 | 0,0,z)$$

$$(2 | 0,0,z)'$$

$$(3) \quad 3'$$

$$(3 | 0,0,z)$$

$$(3 | 0,0,z)'$$

$$(3 | 0,0,z)'$$

For $1'$ set

$$(1) \quad 1'$$

$$(1 | 0,0,0)'$$

$$(1 | 0,0,0)'$$

$$(2) \quad 3'$$

$$(2 | 0,0,z)$$

$$(2 | 0,0,z)'$$

$$(3) \quad 3'$$

$$(3 | 0,0,z)$$

$$(3 | 0,0,z)'$$

$$(3 | 0,0,z)'$$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); 1'.

Positions

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<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry.</th>
<th>Coordinates</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>3 d</td>
<td>11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) y,x-y,z [0,0,0]</td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>1 c</td>
<td>3..1'</td>
<td>2/3,1/3,z [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 b</td>
<td>3..1'</td>
<td>1/3,2/3,z [0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>1 a</td>
<td>3..1'</td>
<td>0,0,z [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p31'  
  \[ \mathbf{a} = \mathbf{a}, \mathbf{b} = \mathbf{b} \]
  Origin at 0,0,z

- Along [1,0,0] p11'  
  \[ \mathbf{a} = \mathbf{c}, \mathbf{b} = (\mathbf{a} + 2\mathbf{b})/2 \]
  Origin at x,0,0

- Along [2,1,0] p11'  
  \[ \mathbf{a} = \mathbf{c}, \mathbf{b} = \mathbf{b}/2 \]
  Origin at x,x/2,0
Origin on 3

Asymmetric unit

$$0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq 1; \quad x \leq \frac{1+y}{2}; \quad y \leq \min(1-x,(1+x)/2)$$

Vertices

$$\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1 & \quad 1/3,2/3,1 & \quad 0,1/2,1
\end{align*}$$

Symmetry Operations

For (0,0,0) +set

$$(1) \; 1 \quad (2) \; 3^* \quad 0,0,z \quad (3) \; 3^* \quad 0,0,z \quad (3_z^3) \quad 0,0,0$$

For (0,0,1)’ +set

$$(1) \; t'(0,0,1) \quad (2) \; 3' \; (0,0,1) \; 0,0,z \quad (3) \; 3' \; (0,0,1) \; 0,0,z \quad (3_z^3) \; (0,0,1)'$$
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2).

Positions

<table>
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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
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<tbody>
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<tr>
<td>6 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td>2 c 3..</td>
<td>2/3,1/3,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 b 3..</td>
<td>1/3,2/3,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 a 3..</td>
<td>0,0,z [0,0,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31' Along [1,0,0] p2a 1 Along [2,1,0] p2a 1

a* = a  b* = b  a* = c  b* = (a + 2b)/2  a* = c  b* = b/2

Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
### Symmetry Operations

<table>
<thead>
<tr>
<th>Operation</th>
<th>Symmetry Operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(2) 3* (0,0,1/3) 0,0,z</td>
</tr>
<tr>
<td>(1</td>
<td>0,0,0)</td>
</tr>
<tr>
<td></td>
<td>(3*z</td>
</tr>
<tr>
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<td>(3*z</td>
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</table>

### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 a 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1)</td>
</tr>
<tr>
<td></td>
<td>y-x,y,z+1/3 [v,u-v,w]</td>
<td>(2)</td>
</tr>
<tr>
<td></td>
<td>x+y,x,z+2/3 [u+v,u,w]</td>
<td>(3)</td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin</th>
<th>Projection 1</th>
<th>Projection 2</th>
<th>Projection 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>$a^* = a$</td>
<td>$b^* = b$</td>
<td></td>
</tr>
<tr>
<td>$a^* = a$</td>
<td>$b^* = b$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>$a^* = c$</td>
<td>$b^* = (a + 2b)/2$</td>
<td>$a^* = c$</td>
</tr>
<tr>
<td></td>
<td>$b^* = c$</td>
<td></td>
<td>$b^* = b/2$</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
<td></td>
<td>Origin at x,x/2,0</td>
</tr>
<tr>
<td>Along [2,1,0]</td>
<td>$a^* = c$</td>
<td>$b^* = b/2$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$b^* = c$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on 3,1'

Asymmetric unit

\[
\begin{array}{cccc}
0 \leq x \leq 1; & 0 \leq y \leq 1; & 0 \leq z \leq 1/3 \\
Vertices & 0,0,0 & 1,0,0 & 1,1,0 & 0,1,0 \\
& 0,0,1/3 & 1,0,1/3 & 1,1,1/3 & 0,1,1/3 \\
\end{array}
\]

Symmetry Operations

For 1 + set

(1) \( t(1,0,0) \)

(2) \( t(0,0,1/3) \)

(3) \( t(0,0,2/3) \)

For 1' + set

(1) \( t(1,0,0)' \)

(2) \( t(0,0,1/3)' \)

(3) \( t(0,0,2/3)' \)

Generators selected

(1); \( t(1,0,0) \); \( t(0,1,0) \); \( t(0,0,1) \); (2); \( 1' \).
Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
<td>a</td>
<td>11'</td>
</tr>
</tbody>
</table>

3          |   |     |

| 1 | x,y,z [0,0,0] | 2 | y-x,y,z+1/3 [0,0,0] | 3 | x+y,x,z+2/3 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1]  p31'  Along [1,0,0]  p11'  Along [2,1,0]  p11'

a* = a  b* = b  a* = c  b* = (a + 2b)/2  a* = c  b* = b/2

Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
Origin on $3_2$

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/3$

Vertices 0,0,0 1,0,0 1,1,0 0,1,0 0,0,1/3 1,0,1/3 1,1,1/3 0,1,1/3

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) $3' (0,0,1/3)$ 0,0,z
    $(3_z |0,0,1/3')$

(3) $3' (0,0,2/3)$ 0,0,z
    $(3_z^{-1} |0,0,2/3')$

For (0,0,1)' + set

(1) $t' (0,0,1)$
    (1|0,0,1)'

(2) $3' (0,0,4/3)$ 0,0,z
    $(3_z |0,0,4/3')$

(3) $3' (0,0,5/3)$ 0,0,z
    $(3_z^{-1} |0,0,5/3')$

Generators selected $(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).
Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>a</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z+1/3 [v,u+v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31'

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

Along [1,0,0] p2x1 1

\[ a^* = c \quad b^* = (a + 2b)/2 \]

Origin at x,0,0

Along [2,1,0] p2x1 1

\[ a^* = c \quad b^* = b/2 \]

Origin at x,x/2,0
Origin on 3

Asymmetric unit
\[
\begin{array}{ccc}
0 \leq x \leq 1; & 0 \leq y \leq 1; & 0 \leq z \leq 1/3 \\
\end{array}
\]

Vertices
\[
\begin{array}{cccc}
0,0,0 & 1,0,0 & 1,1,0 & 0,1,0 \\
0,0,1/3 & 1,0,1/3 & 1,1,1/3 & 0,1,1/3 \\
\end{array}
\]

Symmetry Operations
\[
\begin{align*}
(1) & 1 \\
(2) & 3^* (0,0,2/3) \\
(3) & 3^* (0,0,1/3) \\
\end{align*}
\]

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{align*}
3 & \text{ a 1} \\
(1) & x,y,z [u,v,w] \\
(2) & \bar{y},x-y,z+2/3 [\bar{v},u-v,w] \\
(3) & x+y,\bar{x},z+1/3 [u+v,\bar{u},w] \\
\end{align*}
\]

145.1.1237 - 1 - 2655
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>p3</th>
<th>p1</th>
<th>p1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>(a^* = a)</td>
<td>(a^* = c)</td>
<td>(a^* = c)</td>
</tr>
<tr>
<td></td>
<td>(b^* = b)</td>
<td>(b^* = (a + 2b)/2)</td>
<td>(b^* = b/2)</td>
</tr>
<tr>
<td>Origin</td>
<td>at 0,0,z</td>
<td>at x,0,0</td>
<td>at x,x/2,0</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
Origin on $3_1'$

Asymmetric unit $\begin{align*} &0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3 \\
&\text{Vertices} \quad 0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0 \\
&\quad 0,0,1/3 \quad 1,0,1/3 \quad 1,1,1/3 \quad 0,1,1/3 \end{align*}$

Symmetry Operations

For $1 +$ set

\begin{align*}
(1) \ 1 \\
(1 \ 0,0,0)
\end{align*}

$\begin{align*}
(2) \ 3' \ (0,0,2/3) \quad 0,0,z \\
(3) \ 3' \ (0,0,1/3) \quad 0,0,z
\end{align*}$

For $1' +$ set

\begin{align*}
(1) \ 1' \\
(1 \ 0,0,0')
\end{align*}

$\begin{align*}
(2) \ 3' \ (0,0,2/3) \quad 0,0,z \\
(3) \ 3' \ (0,0,1/3) \quad 0,0,z
\end{align*}$

Generators selected $\begin{align*}
(1) \ : t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ (2) \ : 1'.
\end{align*}$
Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
<td>1'</td>
<td>a</td>
</tr>
</tbody>
</table>

3 a 11' 
(1) x,y,z [0,0,0] 
(2) y,x-y,z+2/3 [0,0,0] 
(3) x+y,x,z+1/3 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p31' 
\( a' = a \) \( b' = b \) 
Origin at 0,0,z

Along [1,0,0] p11' 
\( a' = c \) \( b' = (a + 2b)/2 \) 
Origin at x,0,0

Along [2,1,0] p11' 
\( a' = c \) \( b' = b/2 \) 
Origin at x,x/2,0
Origin on $3_1$

Asymmetric unit $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$
$0,0,1/3 \quad 1,0,1/3 \quad 1,1,1/3 \quad 0,1,1/3$

Symmetry Operations

For $(0,0,0) +$ set

1. $t(0,0,0)$
2. $3^* (0,0,2/3) \quad 0,0,z$
3. $3^- (0,0,1/3) \quad 0,0,z$

For $(0,0,1)' +$ set

1. $t'(0,0,1)$
2. $3^* (0,0,5/3) \quad 0,0,z$
3. $3^- (0,0,4/3) \quad 0,0,z$

Generators selected

1. $t(1,0,0); \ t(0,1,0); \ t'(0,0,1)$; (2).
Continued

145.3.1239

P\textsubscript{2e} \textsubscript{31}

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

\begin{align*}
\text{Multiplicity} & \quad \text{Wyckoff letter} \quad \text{Site Symmetry.} \\
(0,0,0) & + (0,0,1)' + \\
\end{align*}

\begin{align*}
6 & \quad a \quad 1 \\
1 & \quad (1) \quad & \text{x},y,z \ [u,v,w] \\
2 & \quad (2) \quad & \text{y},x-y,z+2/3 \ [v,u-v,w] \\
3 & \quad (3) \quad & \text{x}+y,x,z+1/3 \ [u-v,u,w] \\
\end{align*}

Symmetry of Special Projections

Along [0,0,1] \quad p31'

\begin{align*}
\text{a} & = \text{a} \quad \text{b} & = \text{b} \\
\text{Origin at } 0,0,0 & \quad \text{Origin at } x,0,0 \\
\end{align*}

Along [1,0,0] \quad p_{2a}.1

\begin{align*}
\text{a} & = c \quad \text{b} & = (\text{a} + \text{2b})/2 \\
\text{Origin at } 0,0,0 & \quad \text{Origin at } x,0,0 \\
\end{align*}

Along [2,1,0] \quad p_{2a}.1

\begin{align*}
\text{a} & = c \quad \text{b} & = \text{b}/2 \\
\text{Origin at } 0,0,0 & \quad \text{Origin at } x,x/2,0 \\
\end{align*}
Origin on 3

**Asymmetric unit**

- \( 0 \leq x \leq \frac{2}{3} \); \( 0 \leq y \leq \frac{2}{3} \); \( 0 \leq z \leq \frac{1}{3} \); \( x \leq \frac{(1+y)}{2} \); \( y \leq \min(1-x,(1+x)/2) \)

**Vertices**

- \((0,0,0)\)
- \((0,0,\frac{1}{3})\)
- \((\frac{1}{2},0,0)\)
- \((\frac{1}{2},0,\frac{1}{3})\)
- \(\frac{2}{3},\frac{1}{3},0\)
- \(\frac{1}{3},\frac{2}{3},0\)
- \(\frac{2}{3},\frac{1}{3},\frac{1}{3}\)
- \(\frac{1}{3},\frac{2}{3},\frac{1}{3}\)
- \(0,\frac{1}{2},0\)
- \(0,\frac{1}{2},\frac{1}{3}\)
Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)  
(2) 3* 0,0,z
(3) 3' 0,0,z
(3z | 0,0,0)  
(3z' | 0,0,0)

For (2/3,1/3,1/3) + set

(1) t (2/3,1/3,1/3)
(1 | 2/3,1/3,1/3)  
(2) 3* (0,0,1/3) 1/3,1/3,z
(3) 3' (0,0,1/3) 1/3,0,z
(3z | 2/3,1/3,1/3)  
(3z' | 2/3,1/3,1/3)

For (1/3,2/3,2/3) + set

(1) t (1/3,2/3,2/3)
(1 | 1/3,2/3,2/3)  
(2) 3* (0,0,2/3) 0,1/3,z
(3) 3' (0,0,2/3) 1/3,1/3,z
(3z | 1/3,2/3,2/3)  
(3z' | 1/3,2/3,2/3)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>9</td>
<td>b</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-z [v,u-w,v]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,z [u+v,u+w]</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p3</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a - 2b + c)/3</td>
<td>b* = (a + 2b)/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c/3</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 31'
Symmetry Operations

For (0,0,0) + set

\[(1) \text{ t } (2) \text{ t' } (3) \text{ t' } \]
\[(1,0,0) \quad (0,0,z) \quad (0,0,z) \]

For (2/3,1/3,1/3) + set

\[(1) \text{ t' } (2) \text{ t'} (3) \text{ t'} \]
\[(2/3,1/3,1/3) \quad (0,0,1/3) \quad (0,0,1/3) \]

For (1/3,2/3,2/3) + set

\[(1) \text{ t' } (2) \text{ t'} (3) \text{ t'} \]
\[(1/3,2/3,2/3) \quad (0,0,2/3) \quad (0,0,2/3) \]

For (0,0,0)' + set

\[(1) \text{ t' } (2) \text{ t' } (3) \text{ t'} \]
\[(0,0,0)' \quad (0,0,0)' \quad (0,0,0)' \]

Generators selected

\(1); \text{ t}(1,0,0); \text{ t}(0,1,0); \text{ t}(0,0,1); \text{ t}(2/3,1/3,1/3);(2);1'.\)

Positions

\begin{array}{cccc}
\text{Multiplicity,} & \text{Wyckoff letter,} & \text{Site Symmetry.} \\
9 & b & 11' & \text{ (1) x,y,z [0,0,0] (2) } y,x-y,z [0,0,0] (3) x+y,x,z [0,0,0] \\
3 & a & 3..1' & 0,0,z [0,0,0] \\
\end{array}

Symmetry of Special Projections

Along [0,0,1] p31' \quad \text{Along [1,0,0] p11' \quad Along [2,1,0] p11'}
\[a^* = a \quad b^* = b \quad a^* = (-a - 2b + c)/3 \quad b^* = (a + 2b)/2 \quad a^* = c/3 \quad b^* = b/2 \]
Origin at 0,0,z \quad \text{Origin at x,0,0} \quad \text{Origin at x,x/2,0}
Origin on 3

Asymmetric unit: 

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/3; \quad x \leq (1+y)/2; \quad y \leq \min(1-x, (1+x)/2) \]

Vertices:
- \(0,0,0\)
- \(0,0,1/3\)
- \(1/2,0,0\)
- \(1/2,0,1/3\)
- \(2/3,1/3,0\)
- \(2/3,1/3,1/3\)
- \(1/3,2/3,0\)
- \(1/3,2/3,1/3\)
- \(0,1/2,0\)
- \(0,1/2,1/3\)
Continued

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & & 1 & & (2) & & 3' & & 0,0,z & & (3) & & 3' & & 0,0,z \\
(1') & & (0,0,0) & & (3_z) & & 0,0,0 & & (3_z') & & 0,0,0
\end{align*}
\]

For \((2/3,1/3,1/3)' + \) set

\[
\begin{align*}
(1') & & t'(2/3,1/3,1/3) & & (2) & & 3' & & (0,0,1/3) & & (3) & & 3' & & (0,0,1/3) & & 1/3,0,z \\
(1') & & (2/3,1/3,1/3)' & & (3_z) & & 2/3,1/3,1/3' & & (3_z') & & 2/3,1/3,1/3'
\end{align*}
\]

For \((1/3,2/3,2/3) + \) set

\[
\begin{align*}
(1) & & t(1/3,2/3,2/3) & & (2) & & 3' & & (0,0,2/3) & & (3) & & 3' & & (0,0,2/3) & & 1/3,1/3,z \\
(1') & & (1/3,2/3,2/3) & & (3_z) & & 1/3,2/3,2/3 & & (3_z') & & 1/3,2/3,2/3
\end{align*}
\]

Generators selected

\(1); \(t(1,0,0); \ t(0,1,0); \ t(0,0,1); \ t'(2/3,1/3,1/3); \(2).\)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>b</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>3..</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0) + (2/3,1/3,1/3)' + (1/3,2/3,2/3) + (1/3,2/3,2/3) + )</td>
</tr>
<tr>
<td>((1) x,y,z \ [u,v,w] \quad (2) y-x,y,z \ [v-u,v,w] \quad (3) x+y,x,z \ [u+v,u,w] )</td>
</tr>
<tr>
<td>(0,0,z \ [0,0,w] )</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along \([0,0,1] \quad p31' \)
  - \(a^* = a \quad b^* = b \)
  - Origin at \(0,0,z \)

- Along \([1,0,0] \quad p_{31} \quad p_{31}^{-1} \)
  - \(a^* = (a + 2b)/2 \quad b^* = (a + 2b)/2 \)
  - Origin at \(x,0,0 \)

- Along \([2,1,0] \quad p_{2a} \quad p_{2a}^{-1} \)
  - \(a^* = c/3 \quad b^* = b/2 \)
  - Origin at \(x,x/2,0 \)
Origin on $\overline{3}$

Asymmetric unit: $0 \leq x \leq 2/3$; $0 \leq y \leq 2/3$; $0 \leq z \leq 1/2$; $x \leq (1+y)/2$; $y \leq \min(1-x,(1+x)/2)$

Vertices:
- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/2$
- $1/2,0,1/2$
- $2/3,1/3,1/2$
- $1/3,2/3,1/2$
- $0,1/2,1/2$

Symmetry Operations:

1. $1$
2. $3^+ 0,0,z$
3. $3^- 0,0,z$
4. $\overline{1}$
5. $3^+ 0,0,z; 0,0,0$
6. $3^- 0,0,z; 0,0,0$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 g 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y ,x-y,z [v,u-v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) x ,y ,z [u,v,w]</td>
<td>(5) y,x +y,z [v,u-v,w]</td>
<td></td>
</tr>
<tr>
<td>3 f 1</td>
<td>1/2,0,1/2 [u,v,w]</td>
<td>0,1/2,1/2 [v,u-v,w]</td>
<td></td>
</tr>
<tr>
<td>3 e 1</td>
<td>1/2,0,0 [u,v,w]</td>
<td>0,1/2,0 [v,u-v,w]</td>
<td></td>
</tr>
<tr>
<td>2 d 3</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 c 3</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>1 b 3</td>
<td>0,0,1/2 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a 3</td>
<td>0,0,0 [0,0,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6'</th>
<th>Along [1,0,0]</th>
<th>p2'11</th>
<th>Along [2,1,0]</th>
<th>p2'11</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a  b* = b</td>
<td>a* = c b* = (a + 2b)/2</td>
<td>a* = c b* = b/2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on $\overline{3}1'$

Asymmetric unit

$$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$$

Vertices

$$0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0$$
$$0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2 \quad 1/3,2/3,1/2 \quad 0,1/2,1/2$$

Symmetry Operations

For $1$ +set

(1) $1$

(1|0,0,0)

(2) $3^z \cdot 0,0,z$

(3 $\overline{3}$ $\cdot 0,0,z$

(3 $\overline{z}$ $\cdot 0,0,z$

(1 $\cdot 0,0,0$)

(4) $\overline{1}$

(1 $\overline{1}$|0,0,0)

(5) $\overline{3}^z \cdot 0,0,z; \quad 0,0,0$

(6 $\overline{3}$ $\cdot 0,0,z; \quad 0,0,0$

(3 $\overline{z}$ $\cdot 0,0,0$)

For $1'$ +set

(1) $1'$

(1|0,0,0')

(2) $3^z \cdot 0,0,z$

(3 $\overline{3}$ $\cdot 0,0,z$

(3 $\overline{z}$ $\cdot 0,0,z$

(1 $\cdot 0,0,0$)

(4) $\overline{1}'$

(1 $\overline{1}$|0,0,0')

(5) $\overline{3}^z \cdot 0,0,z; \quad 0,0,0$

(6 $\overline{3}$ $\cdot 0,0,z; \quad 0,0,0$

(3 $\overline{z}$ $\cdot 0,0,0$)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 g 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z [0,0,0]</td>
</tr>
<tr>
<td>3 f 1'</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 e 1'</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 d 3..1'</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>2 c 3..1'</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>1 b 3..1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a 3..1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p61'</th>
<th>Along [1,0,0] p2111'</th>
<th>Along [2,1,0] p2111'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = c b* = (a + 2b)/2</td>
<td>a* = c b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin on $\overline{3}'$

Asymmetric unit

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2 & \quad 0,1/2,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 & \quad (2) & \quad 3^+ & \quad 0,0,z & \quad 3^- & \quad 0,0,z \\
(1|0,0,0) & \quad (3_z|0,0,0) & \quad (3_z^{-1}|0,0,0) & \quad (3_z^{-1}|0,0,0)
\end{align*}
\]

\[
\begin{align*}
(4) & \quad \overline{1} & \quad (5) & \quad \overline{3}^+ & \quad 0,0,z; \quad 0,0,0 & \quad \overline{3}^- & \quad 0,0,z; \quad 0,0,0 \\
(1|0,0,0) & \quad (3_z|0,0,0) & \quad (3_z^{-1}|0,0,0) & \quad (3_z^{-1}|0,0,0)
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>g</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>f</td>
<td>1/2,0,1/2</td>
</tr>
<tr>
<td>3</td>
<td>e</td>
<td>1,0,0</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>1/3,2/3,z</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>0,0,z</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>0,0,1/2</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>0,0,0</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p6

\[
a^* = a^* = b^* = b
\]

Origin at 0,0,z

Along [1,0,0]  p211

\[
a^* = c^* = (a + 2b)/2
\]

Origin at x,0,0

Along [2,1,0]  p211

\[
a^* = c^* = b^* = b/2
\]

Origin at x,x/2,0
Origin on $\overline{3}$

Asymmetric unit 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; 0 ≤ z ≤ 1/2; x ≤ (1+y)/2; y ≤ min(1-x,(1+x)/2)

Vertices 0,0,0 1/2,0,0 2/3,1/3,0 1/3,2/3,0 0,1/2,0
0,0,1/2 1/2,0,1/2 2/3,1/3,1/2 1/3,2/3,1/2 0,1/2,1/2

Symmetry Operations

For (0,0,0) + set
(1) $\overline{1}$
(1 | 0,0,0)
(2) $3^+$ 0,0,z
(3) $3^-$ 0,0,z
(3 | 0,0,0)
(3 | 0,0,0)
(3 | 0,0,0)
(3 | 0,0,0)
(3 | 0,0,0)
(3 | 0,0,0)
(3 | 0,0,0)
(3 | 0,0,0)
(3 | 0,0,0)

For (0,0,1)' + set
(1) $t'$ (0,0,1)
(1 | 0,0,1)'
(2) $3^+' (0,0,1) 0,0,z$
(3) $3^+ (0,0,1) 0,0,z$
(3 | 0,0,1)'
(3 | 0,0,1)'

147.4.1246 - 1 - 2676
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions  

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>g 1</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(0,0,1)’ +</td>
</tr>
<tr>
<td>6</td>
<td>f 1</td>
<td>1/2,0,1/2</td>
</tr>
<tr>
<td>6</td>
<td>e 1</td>
<td>0,1/2,0</td>
</tr>
<tr>
<td>4</td>
<td>d 3</td>
<td>1/3,2/3,z</td>
</tr>
<tr>
<td>4</td>
<td>c 3</td>
<td>0,0,z</td>
</tr>
<tr>
<td>2</td>
<td>b 3’</td>
<td>0,0,1/2</td>
</tr>
<tr>
<td>2</td>
<td>a 3’</td>
<td>0,0,0</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p61’  
\[a^* = a \quad b^* = b\]
Origin at 0,0,z

Along [1,0,0]  p_{2a'} 211  
\[a^* = c \quad b^* = (a + 2b)/2\]
Origin at x,0,1/2

Along [2,1,0]  p_{2a'} 211  
\[a^* = c \quad b^* = b/2\]
Origin at x,x/2,1/2
Origin on $\overline{3}$

**Asymmetric unit**

$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq (1+y)/2; \quad y \leq \min(1-x, (1+x)/2)$

**Vertices**

- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/3,2/3,0
- 0,1/2,0
- 0,0,1/6
- 1/2,0,1/6
- 2/3,1/3,1/6
- 1/3,2/3,1/6
- 0,1/2,1/6
Symmetry Operations

For (0,0,0) + set

(1) 1
  (1) [0,0,0]

(2) 3* 0,0,z
    (3) 3* 0,0,z
    (3_2[0,0,0])
    (3_2[-1][0,0,0])

(4) T
    (T) [0,0,0]

(5) 3* 0,0,z; 0,0,0
    (3_2[0,0,0])
    (3_2[-1][0,0,0])

For (2/3,1/3,1/3) + set

(1) t (2/3,1/3,1/3)
   (1) [2/3,1/3,1/3]

(2) 3* (0,0,1/3) 1/3,1/3,z
    (3) 3* (0,0,1/3) 1/3,0,z
    (3_2[2/3,1/3,1/3])
    (3_2[-1][2/3,1/3,1/3])

(4) T 1/3,1/6,1/6
    (T) [1/3,1/6,1/6]

(5) 3* 1/3,-1/3,z; 1/3,-1/3,1/6
    (3_2[2/3,1/3,1/3])
    (3_2[-1][2/3,1/3,1/3])

For (1/3,2/3,2/3) + set

(1) t (1/3,2/3,2/3)
   (1) [1/3,2/3,2/3]

(2) 3* (0,0,2/3) 0,1/3,z
    (3) 3* (0,0,2/3) 1/3,1/3,z
    (3_2[1/3,2/3,2/3])
    (3_2[-1][1/3,2/3,2/3])

(4) T 1/6,1/3,1/3
    (T) [1/6,1/3,1/3]

(5) 3* 2/3,1/3,z; 2/3,1/3,1/3
    (3_2[1/3,2/3,2/3])
    (3_2[-1][1/3,2/3,2/3])

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>f</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>9</td>
<td>e</td>
<td>(2/3,1/3,1/3)</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>(1/3,2/3,2/3)</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>(1/3,1/6,1/6)</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1], p6'  
Along [1,0,0], p2'11  
Along [2,1,0], p2'11  

a* = (2a + b)/3  
b* = (-a + b)/3  
a* = (-a - 2b + c)/3  
b* = (a + 2b)/2  
a* = c/3  
b* = b/2  
Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x/2,0
Origin on $\overline{3}1'$

<table>
<thead>
<tr>
<th>Asymmetric unit</th>
<th>Vertices</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0 \leq x \leq 2/3$; $0 \leq y \leq 2/3$; $0 \leq z \leq 1/6$; $x \leq (1+y)/2$; $y \leq \min(1-x,(1+x)/2)$</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td></td>
<td>$1/2,0,0$</td>
</tr>
<tr>
<td></td>
<td>$2/3,1/3,0$</td>
</tr>
<tr>
<td></td>
<td>$1/3,2/3,0$</td>
</tr>
<tr>
<td></td>
<td>$0,1/2,0$</td>
</tr>
<tr>
<td>$0,0,1/6$</td>
<td>$1/2,0,1/6$</td>
</tr>
<tr>
<td>$2/3,1/3,1/6$</td>
<td>$1/3,2/3,1/6$</td>
</tr>
<tr>
<td>$0,1/2,1/6$</td>
<td>$0,1/2,1/6$</td>
</tr>
</tbody>
</table>
### Symmetry Operations

#### For \((0,0,0)\) + set

<table>
<thead>
<tr>
<th>(1) (1)</th>
<th>(2) (3') 0,0,z</th>
<th>(3) (3') 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1</td>
<td>0,0,0))</td>
<td>((3,2,0,0,0))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) (\bar{1})</th>
<th>(5) (3') 0,0,z</th>
<th>(6) (3') 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{1}</td>
<td>0,0,0))</td>
<td>((3,2,0,0,0))</td>
</tr>
</tbody>
</table>

#### For \((2/3,1/3,1/3)\) + set

<table>
<thead>
<tr>
<th>(1) (t) ((2/3,1/3,1/3))</th>
<th>(2) (3') ((0,0,1/3)) 1/3,1/3,z</th>
<th>(3) (3') ((0,0,1/3)) 1/3,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1</td>
<td>2/3,1/3,1/3))</td>
<td>((3,2,0,0,0))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) (\bar{1}) (1/3,1/6,1/6)</th>
<th>(5) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
<th>(6) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{1}</td>
<td>2/3,1/3,1/3))</td>
<td>((3,2,0,0,0))</td>
</tr>
</tbody>
</table>

#### For \((1/3,2/3,2/3)\) + set

<table>
<thead>
<tr>
<th>(1) (t) ((1/3,2/3,2/3))</th>
<th>(2) (3') ((0,0,2/3)) 0,1/3,z</th>
<th>(3) (3') ((0,0,2/3)) 1/3,1/3,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1</td>
<td>1/3,2/3,2/3))</td>
<td>((3,2,0,0,0))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) (\bar{1}) (1/3,1/6,1/6)</th>
<th>(5) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
<th>(6) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{1}</td>
<td>1/3,2/3,2/3))</td>
<td>((3,2,0,0,0))</td>
</tr>
</tbody>
</table>

#### For \((0,0,0)\)' + set

<table>
<thead>
<tr>
<th>(1) (1')</th>
<th>(2) (3') 0,0,z</th>
<th>(3) (3') 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1</td>
<td>0,0,0)')</td>
<td>((3,2,0,0,0)')</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) (\bar{1}')</th>
<th>(5) (3') 0,0,z</th>
<th>(6) (3') 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{1}</td>
<td>0,0,0)')</td>
<td>((3,2,0,0,0)')</td>
</tr>
</tbody>
</table>

#### For \((2/3,1/3,1/3)\)' + set

<table>
<thead>
<tr>
<th>(1) (t) ((2/3,1/3,1/3)')</th>
<th>(2) (3') ((0,0,1/3)) 1/3,1/3,z</th>
<th>(3) (3') ((0,0,1/3)) 1/3,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1</td>
<td>2/3,1/3,1/3)')</td>
<td>((3,2,0,0,0)')</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) (\bar{1}) (1/3,1/6,1/6)</th>
<th>(5) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
<th>(6) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{1}</td>
<td>2/3,1/3,1/3)')</td>
<td>((3,2,0,0,0)')</td>
</tr>
</tbody>
</table>

#### For \((1/3,2/3,2/3)\)' + set

<table>
<thead>
<tr>
<th>(1) (t) ((1/3,2/3,2/3)')</th>
<th>(2) (3') ((0,0,2/3)) 0,1/3,z</th>
<th>(3) (3') ((0,0,2/3)) 1/3,1/3,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1</td>
<td>1/3,2/3,2/3)')</td>
<td>((3,2,0,0,0)')</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) (\bar{1}) (1/3,1/6,1/6)</th>
<th>(5) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
<th>(6) (3') (-1/3,-1/3,z) 1/3,1/3,1/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{1}</td>
<td>1/3,2/3,2/3)')</td>
<td>((3,2,0,0,0)')</td>
</tr>
</tbody>
</table>

Generators selected  
(1); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(2/3,1/3,1/3)\); (2); (4); \(1'\).
Continued

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>f</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(0,0,0)' +</td>
<td></td>
<td>(2) y,x-y,z [0,0,0]</td>
</tr>
<tr>
<td>(2/3,1/3,1/3) +</td>
<td></td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>(2/3,1/3,1/3)' +</td>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(1/3,2/3,2/3) +</td>
<td></td>
<td>(5) y,x+y,z [0,0,0]</td>
</tr>
<tr>
<td>(1/3,2/3,2/3)' +</td>
<td></td>
<td>(6) x-y,x,z [0,0,0]</td>
</tr>
</tbody>
</table>

18 f 11' (1) x,y,z [0,0,0] (2) y,x-y,z [0,0,0] (3) x+y,x,z [0,0,0]

9 e 1/2,0,0 [0,0,0] 0,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0]

9 d 1/2,0,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]

6 c 0,0,z [0,0,0] 0,0,z [0,0,0]

1 a 0,0,1/2 [0,0,0]

1 b 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p6' Along [1,0,0] p2111' Along [2,1,0] p2111'

a* = (2a + b)/3 b* = (-a + b)/3 a* = (-a - 2b + c)/3 b* = (a + 2b)/2

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0

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Continued
Origin on \( \bar{3} \)

**Asymmetric unit**

\[
0 \leq x < 2/3; \quad 0 \leq y < 2/3; \quad 0 \leq z < 1/6; \quad x < (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)
\]

**Vertices**

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>2/3,1/3,0</th>
<th>1/3,2/3,0</th>
<th>0,1/2,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,1/6</td>
<td>1/2,0,1/6</td>
<td>2/3,1/3,1/6</td>
<td>1/3,2/3,1/6</td>
<td>0,1/2,1/6</td>
<td></td>
</tr>
</tbody>
</table>
Symmetry Operations

For (0,0,0) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>3'</td>
</tr>
<tr>
<td>3</td>
<td>3'</td>
</tr>
<tr>
<td>4</td>
<td>T</td>
</tr>
<tr>
<td>5</td>
<td>3'</td>
</tr>
<tr>
<td>6</td>
<td>3'</td>
</tr>
</tbody>
</table>

For (2/3,1/3,1/3) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>t</td>
</tr>
<tr>
<td>2</td>
<td>3'</td>
</tr>
<tr>
<td>3</td>
<td>3'</td>
</tr>
<tr>
<td>4</td>
<td>T</td>
</tr>
<tr>
<td>5</td>
<td>3'</td>
</tr>
<tr>
<td>6</td>
<td>3'</td>
</tr>
</tbody>
</table>

For (1/3,2/3,2/3) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>t</td>
</tr>
<tr>
<td>2</td>
<td>3'</td>
</tr>
<tr>
<td>3</td>
<td>3'</td>
</tr>
<tr>
<td>4</td>
<td>T</td>
</tr>
<tr>
<td>5</td>
<td>3'</td>
</tr>
<tr>
<td>6</td>
<td>3'</td>
</tr>
</tbody>
</table>

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)</td>
<td>18</td>
<td>(0,0,0) + x,y,z [u,v,w] (2) y, x-y,z [v,u,v,w] (3) x+y, x, z [u+v,u,w]</td>
</tr>
<tr>
<td>(2/3,1/3,1/3)</td>
<td>9</td>
<td>(2/3,1/3,1/3) + (1/2,0,0) [0,0,0] (5) y, x+z [v,u+v,w] (6) x-y, z [u-v,u,w]</td>
</tr>
<tr>
<td>(1/3,2/3,2/3)</td>
<td>6</td>
<td>(1/3,2/3,2/3) + 0,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1], p6

<table>
<thead>
<tr>
<th>a*</th>
<th>b*</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2a + b)/3</td>
<td>(-a + b)/3</td>
<td>0,0,z</td>
</tr>
</tbody>
</table>

Along [1,0,0], p211

<table>
<thead>
<tr>
<th>a*</th>
<th>b*</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-a - 2b + c)/3</td>
<td>(a + 2b)/2</td>
<td>x,0,0</td>
</tr>
</tbody>
</table>

Along [2,1,0], p211

<table>
<thead>
<tr>
<th>a*</th>
<th>b*</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>c/3</td>
<td>b/2</td>
<td>x,x/2,0</td>
</tr>
</tbody>
</table>
Origin on $\overline{3}$

**Asymmetric unit**

- $0 \leq x \leq 2/3$;
- $0 \leq y \leq 2/3$;
- $0 \leq z \leq 1/6$;
- $x \leq (1+y)/2$;
- $y \leq \min(1-x, (1+x)/2)$

**Vertices**

- $0,0,0$  
- $1/2,0,0$  
- $2/3,1/3,0$  
- $1/3,2/3,0$  
- $0,1/2,0$  
- $0,0,1/6$  
- $1/2,0,1/6$  
- $2/3,1/3,1/6$  
- $1/3,2/3,1/6$  
- $0,1/2,1/6$
Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 3° 0,0,z
(3) 3° 0,0,z
(4) T
(5) 3° 0,0,z; 0,0,0
(6) 3° 0,0,z; 0,0,0

For (2/3,1/3,1/3)' + set

(1) t (2/3,1/3,1/3)
(2) 3°' (0,0,1/3) 1/3,1/3,z
(3) 3°' (0,0,1/3) 1/3,0,z
(4) T'
(5) 3°' 1/3,-1/3,z; 1/3,-1/3,1/6
(6) 3°' 1/3,2/3,z; 1/3,2/3,1/6

For (1/3,2/3,2/3) + set

(1) t (1/3,2/3,2/3)
(2) 3° (0,0,2/3) 0,1/3,z
(3) 3° (0,0,2/3) 1/3,1/3,z
(4) T
(5) 3° 2/3,1/3,z; 2/3,1/3,1/3
(6) 3° -1/3,1/3,z; -1/3,1/3,1/3

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).

Positions

Multiplicity, Coordinates
Wyckoff letter, Site Symmetry.

(0,0,0) + (2/3,1/3,1/3)' + (1/3,2/3,2/3) +

18 f 1  (1) x,y,z [u,v,w]  (2) y,x-y,z [v,u-v,w]  (3) x+y,x,z [u+v,u,w]
(4) x,y,z [u,v,w]  (5) y,x+y,z [v,u-v,w]  (6) x-y,x,z [u,v,u-w]
10 e 1/2,0,0 [u,v,w]  0,1/2,0 [v,u-v,w]  1/2,1,2,0 [u+v,u,w]
9 d 1/2,0,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]
6 c 0,0,z [0,0,w]  0,0,z [0,0,w]
1 b 0,0,1/2 [0,0,0]
1 a 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p61′
a° = (2a + b)/3 b° = (-a + b)/3
Origin at 0,0,z

Along [1,0,0] p211
a° = (-a - 2b + c)/3 b° = (a + 2b)/2
Origin at x,0,1/2

Along [2,1,0] p211
a° = c/3 b° = b/2
Origin at x,x/2,1/2
Origin on 312

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,(1+x)/2) \]

Vertices

\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/3,2/3,0 & & 0,1/2,0 \\
0,0,1/2 & & 1/2,0,1/2 & & 2/3,1/3,1/2 & & 1/3,2/3,1/2 & & 0,1/2,1/2
\end{align*}

Symmetry Operations

\begin{align*}
(1) & & 1 \\
(1\cdot 0,0,0) & & (2) 3^+ & & 0,0,z \\
(3) & & (3_z) & & 0,0,0 \\
(3^{-1}) & & (3^{-1}_z) & & 0,0,0 \\
(4) & & 2 & & x,x,0 \\
(2_3 0,0,0) & & (5) & & x,2x,0 \\
(2_2 0,0,0) & & (6) & & 2x,x,0 \\
(2_1 0,0,0) & & (2_0 0,0,0)
\end{align*}
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>l</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>3</td>
<td>k</td>
<td>(4) (\bar{y},x,z [\bar{v},u,w])</td>
</tr>
<tr>
<td>3</td>
<td>j</td>
<td>x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td>2</td>
<td>i</td>
<td>x,0 [u,u,0]</td>
</tr>
<tr>
<td>2</td>
<td>h</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>g</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>f</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>e</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>d</td>
<td>2/3,1/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>c</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p3m'1
\(\mathbf{a}^* = \mathbf{a}\) \(\mathbf{b}^* = \mathbf{b}\)
Origin at 0,0,z

Along [1,0,0] p1m'1
\(\mathbf{a}^* = \mathbf{c}\) \(\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2\)
Origin at x,0,0

Along [2,1,0] p211
\(\mathbf{a}^* = \mathbf{c}\) \(\mathbf{b}^* = \mathbf{b}/2\)
Origin at x,x/2,0
Origin on 3121'

Asymmetric unit

\begin{align*}
0 & \leq x \leq 2/3; & 0 & \leq y \leq 2/3; & 0 & \leq z \leq 1/2; & x & \leq (1+y)/2; & y & \leq \min(1-x,(1+x)/2) \\
\end{align*}

Vertices

\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/3,2/3,0 & & 0,1/2,0 \\
0,0,1/2 & & 1/2,0,1/2 & & 2/3,1/3,1/2 & & 1/3,2/3,1/2 & & 0,1/2,1/2 \\
\end{align*}

Symmetry Operations

For 1 + set

\begin{align*}
(1) & \ 1 & (2) & 3^+ & 0,0,z & (3) & 3^- & 0,0,z \\
(1' | 0,0,0) & & (3_z | 0,0,0) & & (3_z^- | 0,0,0) & & (3_z^- | 0,0,0) \\
(4) & 2 & x,\bar{x},0 & (5) & 2 & x,2x,0 & (6) & 2 & 2x,x,0 \\
(2_z | 0,0,0) & & (2_z | 0,0,0) & & (2_1 | 0,0,0) & & (2_1 | 0,0,0) \\
\end{align*}

For 1' + set

\begin{align*}
(1) & \ 1' & (2) & 3^+ & 0,0,z & (3) & 3^- & 0,0,z \\
(1' | 0,0,0)' & & (3_z | 0,0,0)' & & (3_z^- | 0,0,0)' & & (3_z^- | 0,0,0)' \\
(4) & 2' & x,\bar{x},0 & (5) & 2' & x,2x,0 & (6) & 2' & 2x,x,0 \\
(2_z | 0,0,0)' & & (2_z | 0,0,0)' & & (2_1 | 0,0,0)' & & (2_1 | 0,0,0)' \\
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>l</td>
<td>11'</td>
</tr>
<tr>
<td>3</td>
<td>k</td>
<td>21'</td>
</tr>
<tr>
<td>2</td>
<td>i</td>
<td>11'</td>
</tr>
<tr>
<td>2</td>
<td>h</td>
<td>31'</td>
</tr>
<tr>
<td>2</td>
<td>g</td>
<td>31'</td>
</tr>
<tr>
<td>1</td>
<td>f</td>
<td>3.21'</td>
</tr>
<tr>
<td>1</td>
<td>e</td>
<td>3.21'</td>
</tr>
<tr>
<td>1</td>
<td>d</td>
<td>3.21'</td>
</tr>
<tr>
<td>1</td>
<td>c</td>
<td>3.21'</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>3.21'</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>3.21'</td>
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</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>+</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>+</td>
<td>(2) y,x-y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x+y,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x-y,w [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>k</td>
<td>x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>j</td>
<td>x,x,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>i</td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>h</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>g</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>f</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>e</td>
<td>2/3,1/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>d</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
</tr>
<tr>
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<td>0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p3m11'  
\[ a^* = a, \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p1m11'  
\[ a^* = c, \quad b^* = (a + 2b)/2 \]
Origin at x,0,0

Along [2,1,0] p2111'  
\[ a^* = c, \quad b^* = b/2 \]
Origin at x,x/2,0
Origin on 312'

Asymmetric unit:

\[
0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,(1+x)/2)
\]

Vertices:

- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/3,2/3,0
- 0,1/2,0
- 0,0,1/2
- 1/2,0,1/2
- 2/3,1/3,1/2
- 1/3,2/3,1/2
- 0,1/2,1/2

Symmetry Operations:

(1) 1
(1 | 0,0,0)

(2) 3^\ast\ 0,0,z
(3_z | 0,0,0)

(3) 3^-\ 0,0,z
(3_z^{-1} | 0,0,0)

(4) 2' \ x,\ x,\ 0
(2_z | 0,0,0)^\prime

(5) 2' \ x,2x,0
(2_z | 0,0,0)^\prime

(6) 2' \ 2x,x,0
(2_z | 0,0,0)^\prime
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
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<th>Site Symmetry</th>
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<td>x,x,1/2 [u,u,w]</td>
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<td>j</td>
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<td>2/3,1/3,z [0,0,w]</td>
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<td>1/3,2/3,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>0,0,0 [0,0,w]</td>
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Symmetry of Special Projections

Along [0,0,1] p3m1  
\[ a^* = a, \ b^* = b \]
Origin at 0,0,z

Along [1,0,0] p1m1  
\[ a^* = c, \ b^* = (a+2b)/2 \]
Origin at x,0,0

Along [2,1,0] p2'11  
\[ a^* = c, \ b^* = b/2 \]
Origin at x,x/2,0
Origin on 312

Asymmetric unit

$$0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,(1+x)/2)$$

Vertices

\[
\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/3,2/3,0 & & 0,1/2,0 \\
0,0,1/2 & & 1/2,0,1/2 & & 2/3,1/3,1/2 & & 1/3,2/3,1/2 & & 0,1/2,1/2
\end{align*}
\]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3' \quad 0,0,z \\
(4) & \quad 2 \quad x,x,0 \\
(5) & \quad 2 \quad x,2x,0 \\
(6) & \quad 2 \quad 2x,x,0
\end{align*}
\]

For (0,0,1)' + set

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(1) & \quad (0,0,1)' \\
(2) & \quad 3' \quad (0,0,1) \quad 0,0,z \\
(3) & \quad 3' \quad (0,0,1) \quad 0,0,z \\
(4) & \quad 2' \quad x,x,1/2 \\
(5) & \quad 2' \quad x,2x,1/2 \\
(6) & \quad 2' \quad 2x,x,1/2
\end{align*}
\]
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions
Multiplicity, Wyckoff letter, Site Symmetry, Coordinates

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<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>1/3,2/3,0 [0,0,0]</td>
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<tr>
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<td>b</td>
<td>3.2'</td>
<td>0,0,1/2 [0,0,w]</td>
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<td>0,0,1/2 [0,0,w]</td>
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<td>0,0,0 [0,0,0]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1] p3m11' 

a* = a b* = b
Origin at 0,0,z

Along [1,0,0] p2a1m1

a* = a b* = (a + 2b)/2
Origin at x,0,0

Along [2,1,0] p2a211

a* = c b* = b/2
Origin at x,x/2,0
Origin on 321

Asymmetric unit  
0 ≤ x ≤ 2/3;  0 ≤ y ≤ 2/3;  0 ≤ z ≤ 1/2;  x ≤ (1+y)/2;  y ≤ min(1-x,(1+x)/2)

Vertices  
0,0,0  1/2,0,0  2/3,1/3,0  1/3,2/3,0  0,1/2,0  0,0,1/2  1/2,0,1/2  2/3,1/3,1/2  1/3,2/3,1/2  0,1/2,1/2

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 3^+ 0,0,z  
(3_z|0,0,0)

(3) 3^- 0,0,z  
(3_z^-|0,0,0)

(4) 2  x,x,0  
(2_xy|0,0,0)

(5) 2  x,0,0  
(2_x|0,0,0)

(6) 2  0,y,0  
(2_y|0,0,0)
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
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<td>6</td>
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<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) (\bar{y},x-y,z [v,u-v,w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) (x+y,x,z [u+\bar{v},\bar{u},w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,(\bar{z}) [v,u,(\bar{w})]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x-y,(\bar{y},z [u-v,\bar{v},w])</td>
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<tr>
<td></td>
<td></td>
<td>(6) (x,x+y,\bar{z} [u,\bar{u}+v,\bar{w}])</td>
</tr>
<tr>
<td>3</td>
<td>f</td>
<td>.2. x,0,1/2 [u,0,0]</td>
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<tr>
<td></td>
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<td>0,x,1/2 [0,u,0]</td>
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<tr>
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<td></td>
<td>(\bar{x},\bar{x},1/2 [\bar{u},\bar{u},0])</td>
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<tr>
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<td>(\bar{x},\bar{x},0 [\bar{u},\bar{u},0])</td>
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<tr>
<td>2</td>
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<td>3.. 1/3,2/3,z [0,0,w]</td>
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<td>3.. 0,0,z [0,0,w]</td>
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<td>0,0,(\bar{z} [0,0,\bar{w}])</td>
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<td>32. 0,0,1/2 [0,0,0]</td>
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<tr>
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<td>32. 0,0,0 [0,0,0]</td>
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</table>

**Symmetry of Special Projections**

- Along [0,0,1] p31m’
  - \(\mathbf{a^*} = \mathbf{a}\)  \(\mathbf{b^*} = \mathbf{b}\) Origin at 0,0,z

- Along [1,0,0] p211
  - \(\mathbf{a^*} = \mathbf{c}\)  \(\mathbf{b^*} = (\mathbf{a} + 2\mathbf{b})/2\) Origin at x,0,0

- Along [2,1,0] p1m’1
  - \(\mathbf{a^*} = \mathbf{c}\)  \(\mathbf{b^*} = \mathbf{b}/2\) Origin at x,x/2,0
Origin on 3211’

Asymmetric unit

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,(1+x)/2)\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0 \]

\[0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2 \quad 1/3,2/3,1/2 \quad 0,1/2,1/2\]

Symmetry Operations

For 1 + set

(1) 1
(1) 0,0,0
(1) 0,0,0

(2) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z

(4) 2  x,x,0
(2)  x,x,0
(2)  x,x,0
(2)  x,x,0
(2)  x,x,0
(2)  x,x,0
(2)  x,x,0
(2)  x,x,0
(2)  x,x,0

(5) 2’ x,0,0
(6) 2’ x,0,0
(6) 2’ x,0,0
(6) 2’ x,0,0
(6) 2’ x,0,0
(6) 2’ x,0,0
(6) 2’ x,0,0
(6) 2’ x,0,0

For 1’ + set

(1) 1’
(1) 0,0,0’
(1) 0,0,0’

(2) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z
(3) 3’ 0,0,z

(4) 2’ x,x,0
(5) 2’ x,x,0
(6) 2’ x,x,0
(6) 2’ x,x,0
(6) 2’ x,x,0
(6) 2’ x,x,0
(6) 2’ x,x,0
(6) 2’ x,x,0

150.2.1256 - 1 - 2701
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2);(4); 1'.

<table>
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<th>Coordinates</th>
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<td>1</td>
<td></td>
</tr>
<tr>
<td>0,0,1/2</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(1)</td>
<td></td>
</tr>
<tr>
<td>a</td>
<td>32.1'</td>
</tr>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>0,0,0</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(1)</td>
<td></td>
</tr>
<tr>
<td>Symmetry of Special Projections</td>
<td></td>
</tr>
<tr>
<td>Along [0,0,1]</td>
<td>p31m1'</td>
</tr>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2111'</td>
</tr>
<tr>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
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<tr>
<td>Along [2,1,0]</td>
<td>p1m11'</td>
</tr>
<tr>
<td>a* = c</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 32'1

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,\frac{(1+x)}{2}) \]

Vertices

\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2 & \quad 0,1/2,1/2
\end{align*}

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(1|0,0,0) & \quad (2) & \quad 3^* & \quad 0,0,z \\
(3z|0,0,0) & \quad (3) & \quad 3^* & \quad 0,0,z \\
(2xy|0,0,0)' & \quad (5) & \quad 2^* & \quad x,0,0 \\
(2x|0,0,0)' & \quad (6) & \quad 2^* & \quad 0,y,0 \\
(2y|0,0,0)' & & & \quad (2y|0,0,0)'
\end{align*}
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>g</td>
<td>1 (1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w] (4) y,x,z [v,u-w]</td>
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<tr>
<td></td>
<td></td>
<td>(5) x-y,y,z [u+v,v,w] (6) x,x+y,z [u,v,w]</td>
</tr>
<tr>
<td>3</td>
<td>f</td>
<td>.2' x,0,1/2 [u,2u,w] 0,x,1/2 [2u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,1/2 [u,u,w]</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
<td>.2' x,0,0 [u,2u,w] 0,x,0 [2u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>3.. 1/3,2/3,z [0,0,w] 2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>3.. 0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>32' 0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>32' 0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m Along [1,0,0] p2'11 Along [2,1,0] p1m1
\[ a^* = a \quad b^* = b \quad a^* = c \quad b^* = (a + 2b)/2 \quad a^* = c \quad b^* = b/2 \]
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
Origin on 321

Asymmetric unit

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2 & \quad 0,1/2,1/2
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(1') & \quad 0,0,0 \\
(2) & \quad 2 \quad x,x,0 \\
(2_{xy}) & \quad (0,0,0) \\
(3) & \quad 3^* \quad 0,0,z \\
(3_z) & \quad 0,0,0 \\
(4) & \quad 2^* \quad x,x,0 \\
(5) & \quad 2_{xy} \quad (0,0,0) \\
(6) & \quad 2 \quad 0,y,0 \\
(2_y) & \quad (0,0,0)
\end{align*}
\]

For \((0,0,1)' + \text{set}\)

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(1') & \quad (0,0,1)' \\
(2) & \quad 3^* \quad (0,0,1) \\
(3_z) & \quad 0,0,1' \\
(3) & \quad 3^* \quad (0,0,1) \\
(3_z) & \quad 0,0,1' \\
(4) & \quad 2^* \quad x,x,1/2 \\
(5) & \quad 2_{xy} \quad (0,0,1)' \\
(6) & \quad 2' \quad 0,y,1/2 \\
(2_y) & \quad (0,0,1)'
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y-y,x,z [v-u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>6</td>
<td>f .2'</td>
<td>x,0,1/2 [u,2u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,x,1/2 [2u,u,w]</td>
</tr>
<tr>
<td>6</td>
<td>g .2</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
<td>4</td>
<td>d 3..</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c 3..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b 32'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 32</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  p31m1'  
\( a^* = a \quad b^* = b \)  
Origin at 0,0,z

Along [1,0,0]  p_{2a}.211  
\( a^* = c \quad b^* = (a + 2b)/2 \)  
Origin at x,0,0

Along [2,1,0]  p_{2a}.1m1  
\( a^* = c \quad b^* = b/2 \)  
Origin at x,x/2,1/2
Origin on 2 [210] at 3,1(1,1,2)

Asymmetric unit

\begin{align*}
\text{Vertices} & \quad 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \\
0,0,0 & \quad 1,0,0 \quad 1,1,0 \quad 0,1,0 \\
0,0,1/6 & \quad 1,0,1/6 \quad 1,1,1/6 \quad 0,1,1/6
\end{align*}

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(23) & \quad x,x,1/3 \\
(23) & \quad 0,0,2/3
\end{align*}

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,1/3 \\
(2) & \quad 0,0,1/3
\end{align*}

\begin{align*}
(3) & \quad 3^- \quad 0,0,2/3 \\
(3) & \quad 0,0,2/3
\end{align*}

\begin{align*}
(4) & \quad 2x,x,1/3 \\
(2) & \quad 0,0,1/3
\end{align*}

\begin{align*}
(5) & \quad 2x,x,0 \\
(2) & \quad 0,0,0
\end{align*}
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z+1/3 [v,u-v,w] (3) x+y,x,z+2/3 [u+v,u,w] (4) y,x,z+2/3 [v,u,w] (5) x+y,y,z+1/3 [u+v,v,w] (6) x,y,z+2/3 [v,u,w]</td>
</tr>
<tr>
<td>3 b 0.2</td>
<td>x,x,5/6 [u,u,0] x,2x,1/6 [u,2u,0] 2x,x,1/2 [2u,u,0]</td>
</tr>
<tr>
<td>3 a 0.2</td>
<td>x,x,1/3 [u,u,0] x,2x,2/3 [u,2u,0] 2x,x,0 [2u,u,0]</td>
</tr>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p3m'1</th>
<th>Along [1,0,0] p1m'1</th>
<th>Along [2,1,0] p211</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a) b^* = b</td>
<td>a^* = c b^* = (a + 2b)/2</td>
<td>a^* = c b^* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,1/6</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin on 21'[210] at 3,1(1,1,2)1'

Asymmetric unit

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{6}\]

Vertices

\[0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0\]

\[0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}\]

Symmetry Operations

For 1 + set

\[(1) \quad 1 \quad (2) \quad 3^* (0,0,1/3) \quad 0,0,z\]

\[(3) \quad 3^* (0,0,2/3) \quad 0,0,z\]

\[(4) \quad 2 \quad x,x,1/3 \quad (2_3|0,0,2/3)\]

\[(5) \quad 2 \quad x,2x,1/6 \quad (2_3|0,0,1/3)\]

\[(6) \quad 2 \quad 2x,x,0\]

For 1' + set

\[(1) \quad 1' \quad (2) \quad 3^* '(0,0,1/3) \quad 0,0,z\]

\[(3) \quad 3^* '(0,0,2/3) \quad 0,0,z\]

\[(4) \quad 2' \quad x,x,1/3 \quad (2_3|0,0,2/3)\]

\[(5) \quad 2' \quad x,2x,1/6 \quad (2_3|0,0,1/3)\]

\[(6) \quad 2' \quad 2x,x,0\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>1 + 1' +</td>
</tr>
<tr>
<td>6 c 1' 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+2/3 [0,0,0]</td>
</tr>
<tr>
<td>3 b ..21'</td>
<td>x,x,5/6 [0,0,0]</td>
</tr>
<tr>
<td>3 a ..21'</td>
<td>x,x,1/3 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p3m11'  
Origin at 0,0,z

Along [1,0,0] p1m11'  
Origin at x,0,1/6

Along [2,1,0] p2111'  
Origin at x,x/2,0

\[ \mathbf{a^*} = \mathbf{a} \quad \mathbf{b^*} = \mathbf{b} \]

\[ \mathbf{a^*} = \mathbf{a} \quad \mathbf{b^*} = (\mathbf{a} + 2\mathbf{b})/2 \]

\[ \mathbf{a^*} = \mathbf{b} \quad \mathbf{b^*} = \mathbf{b}/2 \]
Origin on 2' [210] at 3,1(1,1,2')

Asymmetric unit: 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/6

Vertices: 0,0,0; 1,0,0; 1,1,0; 0,1,0; 0,0,1/6; 1,0,1/6; 1,1,1/6; 0,1,1/6

Symmetry Operations:

1. 1
   1 0,0,0

2. 3' (0,0,1/3) 0,0,z
   (3z) 0,0,1/3

3. 3' (0,0,2/3) 0,0,z
   (3z') 0,0,2/3

4. 2' x,x,1/3
   (2z) 0,0,2/3
   (2z') 0,0,1/3

5. 2' x,2x,1/6
   (2z) 0,0,1/3
   (2z') 0,0,0

6. 2' 2x,x,0
   (2z) 0,0,0
   (2z') 0,0,0

P3\(_{12}'\)

312' Trigonal
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>6</td>
<td>c</td>
<td>(1) x,y,z  [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z+1/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z+2/3 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x+y,y,z+1/3 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,y,z+1/3 [u,v,w]</td>
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</table>

3 b ..2' x,x,5/6 [u,u,w] x,2x,1/6 [u,0,w] 2x,x,1/2 [0,u,w]
3 a ..2' x,x,1/3 [u,u,w] x,2x,2/3 [u,0,w] 2x,x,0 [0,u,w]

Symmetry of Special Projections

Along [0,0,1]  p3m1  Along [1,0,0]  p1m1  Along [2,1,0]  p211
a* = a  b* = b  a* = c  b* = (a + 2b)/2  a* = c  b* = b/2
Origin at 0,0,z  Origin at x,0,1/6  Origin at x,x/2,0
Origin on 2 [210] at $3_2\{1,1,2\}$

Asymmetric unit

$0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq 1/6$

Vertices

<table>
<thead>
<tr>
<th>Vertices</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
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<td>0</td>
<td>1</td>
</tr>
<tr>
<td>0,0,1/6</td>
<td>1</td>
<td>0</td>
<td>1/6</td>
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<tr>
<td>1,0,0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1,0,1/6</td>
<td>0</td>
<td>1</td>
<td>1/6</td>
</tr>
<tr>
<td>1,1,0</td>
<td>1</td>
<td>1</td>
<td>0</td>
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<td>1,1,1/6</td>
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<td>1</td>
<td>1/6</td>
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<tr>
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<td>1</td>
</tr>
<tr>
<td>0,1,1/6</td>
<td>0</td>
<td>0</td>
<td>1/6</td>
</tr>
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</table>

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
2. $3' \ (0,0,1/3)$
3. $3' \ (0,0,2/3)$

For $(0,0,1)'$ + set

1. $t' \ (0,0,1)$
2. $3' \ (0,0,4/3)$
3. $3' \ (0,0,5/3)$

151.4.1262 - 1 - 2713
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

<table>
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<tr>
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<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
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<tbody>
<tr>
<td>12</td>
<td>c</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td>..2'</td>
</tr>
<tr>
<td>6</td>
<td>a</td>
<td>.2</td>
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<td>(0,0,1)' +</td>
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<tr>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) y,x-y,z+1/3 [v,u+v,w]</td>
</tr>
<tr>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td>(4) y,x,z+2/3 [v,u,w]</td>
</tr>
<tr>
<td>(5) x+y,y,z+1/3 [u-v,v,w]</td>
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<td>(6) x,x-y,z [u,u-v,w]</td>
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<tr>
<td>x,x,5/6 [u,u,w]</td>
</tr>
<tr>
<td>x,2x,1/6 [u,0,w]</td>
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<tr>
<td>2x,x,1/2 [0,u,w]</td>
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<tr>
<td>x,x,1/3 [u,u,0]</td>
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<td>2x,x,0 [2u,u,0]</td>
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Symmetry of Special Projections

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<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p3m11'</th>
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<tbody>
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<td>a* = a</td>
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<tr>
<td>b* = b</td>
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<td>Origin at 0,0,z</td>
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<table>
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<tr>
<th>Along [1,0,0]</th>
<th>p2a1m1</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>b* = (a + 2b)/2</td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,1/6</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p2e 211</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td></td>
</tr>
<tr>
<td>b* = b/2</td>
<td></td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2 [110] at 3, (1,1,2) 1

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 & \quad 0,1,0 \\
0,0,1/6 & \quad 1,0,1/6 & \quad 1,1,1/6 & \quad 0,1,1/6
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(1) & \quad (0,0,0) \\
(2) & \quad (0,0,1/3) \\
(2) & \quad (0,0,1/3) \\
(3) & \quad (0,0,2/3) \\
(3) & \quad (0,0,2/3) \\
(4) & \quad (0,0,0) \\
(4) & \quad (2_{xy}|0,0,0) \\
(5) & \quad (0,0,2/3) \\
(5) & \quad (0,0,2/3) \\
(6) & \quad (0,0,1/6) \\
(6) & \quad (0,0,1/6)
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z+1/3 [v-u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x-y,y,z+2/3 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 b .2.</td>
<td>x,0,5/6 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,x,1/6 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [u,u,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 a .2.</td>
<td>x,0,1/3 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,x,2/3 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  p31m'  
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0]  p211  
\[ a^* = c \quad b^* = (a + 2b)/2 \]
Origin at x,0,1/3

Along [2,1,0]  p1m'1  
\[ a^* = c \quad b^* = b/2 \]
Origin at x,x/2,1/6
Asymmetric unit  
0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/6

Vertices  
0,0,0 1,0,0 1,1,0 0,1,0 0,0,1/6 1,0,1/6 1,1,1/6 0,1,1/6

Symmetry Operations

For 1 + set

(1) 1  
(1 | 0,0,0)

(2) 3' (0,0,1/3) 0,0,z
     (3z | 0,0,1/3)

(4) 2 x,x,0  
     (2xy | 0,0,0)

(5) 2 x,0,1/3  
     (2z | 0,0,2/3)

(6) 2 0,y,1/6  
     (2y | 0,0,1/3)

For 1' + set

(1) 1'  
(1 | 0,0,0)'

(2) 3' ' (0,0,1/3) 0,0,z
      (3z' | 0,0,1/3)'

(3) 3' ' (0,0,2/3) 0,0,z
      (3z'' | 0,0,2/3)'

(4) 2' x,x,0  
     (2xy' | 0,0,0)'

(5) 2' x,0,1/3  
     (2z' | 0,0,2/3)'

(6) 2' 0,y,1/6  
     (2y' | 0,0,1/3)'

152.2.1264 - 1 - 2717
Continued

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1'</td>
<td></td>
</tr>
<tr>
<td>6 c 11'</td>
<td>(1) x,y,z [0,0,0] (2) y,x-y,z+1/3 [0,0,0] (3) x+y,x,z+2/3 [0,0,0]</td>
</tr>
<tr>
<td>(4) y,x,z [0,0,0]</td>
<td>(5) x-y,y,z+2/3 [0,0,0]</td>
</tr>
<tr>
<td>(6) x,x+y,z+1/3 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>3 b 0.2.1'</td>
<td>(1) x,0,5/6 [0,0,0] (2) 0,x,1/6 [0,0,0] (3) x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 a 0.2.1'</td>
<td>(1) x,0,1/3 [0,0,0] (2) 0,x,2/3 [0,0,0] (3) x,x,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p31m1'</th>
<th>Along [1,0,0] p2111'</th>
<th>Along [2,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a, b* = b</td>
<td>a* = c, b* = (a + 2b)/2</td>
<td>a* = c, b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,1/3</td>
<td>Origin at x,x/2,1/6</td>
</tr>
</tbody>
</table>
Origin on 2' [110] at 3,(1,1,2') 1

Asymmetric unit

<table>
<thead>
<tr>
<th></th>
<th>0 ≤ x ≤ 1;</th>
<th>0 ≤ y ≤ 1;</th>
<th>0 ≤ z ≤ 1/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices</td>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
</tr>
<tr>
<td></td>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
</tr>
</tbody>
</table>

Symmetry Operations

1. 1
2. 3' (0,0,1/3) 0,0,z
3. 3' (0,0,2/3) 0,0,z
4. 2' x,x,0
5. 2' x,0,1/3
6. 2' 0,y,1/6

152.3.1265 - 1 - 2719
**Generators selected**  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z+1/3 [v-u-v,w] (3) x+y,x,z+2/3 [u+v,u,w] (4) y,x,z [v-u,w] (5) x-y,y,z+2/3 [u-v,u,w] (6) x+y,z+1/3 [u,u,v,w]</td>
</tr>
<tr>
<td>3 b .2'</td>
<td>x,0,5/6 [u,2u,w] 0,x,1/6 [2u,u,w] x,x,1/2 [u,u,w]</td>
</tr>
<tr>
<td>3 a .2'</td>
<td>x,0,1/3 [u,2u,w] 0,x,2/3 [2u,u,w] x,x,0 [u,u,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p31m</th>
<th>Along [1,0,0] p2'11</th>
<th>Along [2,1,0] p1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = c b* = (a + 2b)/2</td>
<td>a* = c b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,1/3</td>
<td>Origin at x,x/2,1/6</td>
</tr>
</tbody>
</table>
Origin on 2 [110] at $3_{2}(1,1,2)$

Asymmetric unit

$0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{6}$

Vertices

- $0,0,0$
- $1,0,0$
- $1,1,0$
- $0,1,0$
- $0,0,\frac{1}{6}$
- $1,0,\frac{1}{6}$
- $1,1,\frac{1}{6}$
- $0,1,\frac{1}{6}$

Symmetry Operations

For $(0,0,0)$ + set

1. $1$
   
   - $(1|0,0,0)$

2. $3^*$ $(0,0,1/3)$ $0,0,z$
   
   - $(3_z|0,0,1/3)^*$

3. $3^*$ $(0,0,2/3)$ $0,0,z$
   
   - $(3_z^-|0,0,2/3)$

For $(0,0,1)^*$ + set

1. $t^*$ $(0,0,1)$
   
   - $(1|0,0,1)^*$

2. $3^*$ $(0,0,4/3)$ $0,0,z$
   
   - $(3_z|0,0,4/3)$

3. $3^*$ $(0,0,5/3)$ $0,0,z$
   
   - $(3_z^-|0,0,5/3)^*$

4. $2^*$ $x,x,1/2$
   
   - $(2_{xy}|0,0,0)$

5. $2^*$ $(0,0,5/6)$ $x,0,1/3$
   
   - $(2|x|0,0,2/3)$

6. $2^*$ $0,y,2/3$
   
   - $(2|y|0,0,4/3)^*$

$P_{2c} \ 3_{2} \ 21$

$3211^*$

Trigonal

152.4.1266

$P_{2c} \ 3_{2} \ 21$
Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>c 1</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>12</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y',x-y,z+1/3 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x-y,y,z+2/3 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,x+y,z+1/3 [u,u-v,w]</td>
</tr>
<tr>
<td>6 b</td>
<td>0,x,5/6 [u,2u,w]</td>
</tr>
<tr>
<td></td>
<td>0,x,1/6 [2u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x-,x,1/2 [u,u,w]</td>
</tr>
<tr>
<td>6 a</td>
<td>x,0,1/3 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,x,2/3 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>x-,x,0 [u,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p31m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a \ b* = b</td>
<td>Origin at 0,0,z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p_2c 211</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c \ b* = (a + 2b)/2</td>
<td>Origin at x,0,1/3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p_2c 1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c \ b* = b/2</td>
<td>Origin at x,x/2,1/6</td>
</tr>
</tbody>
</table>
Origin on 2 [210] at $3_2 1(1,1,2)$

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq 1/6$

Vertices

<table>
<thead>
<tr>
<th></th>
<th>0,0</th>
<th>1,0</th>
<th>1,1</th>
<th>0,1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>,0,0</td>
<td>,0,0</td>
<td>,1,0</td>
<td>,0,1</td>
</tr>
<tr>
<td></td>
<td>,0,1/6</td>
<td>,1,0</td>
<td>,1,1/6</td>
<td>,0,1/6</td>
</tr>
</tbody>
</table>

Symmetry Operations

1. $1$
2. $3^*$ $(0,0,2/3)$, $0,0,z$
3. $3^{-1} (0,0,1/3)$, $0,0,z$
4. $2x,x,1/6$
5. $2x,2x,1/3$
6. $2x,0$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-z,1/3 [v,u-w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z+1/3 [v,u-w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+y,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,x-y,z+2/3 [v,u-w]</td>
</tr>
<tr>
<td>3 b ..2</td>
<td>x,x,1/6 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,2x,5/6 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td>2x,x,1/2 [2u,u,0]</td>
</tr>
<tr>
<td>3 a ..2</td>
<td>x,x,2/3 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,2x,1/3 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td>2x,x,0 [2u,u,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p3m'1</th>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
<th>Along [2,1,0]</th>
<th>p211</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
<td>a* = c b* = (a + 2b)/2</td>
<td></td>
<td>a* = c b* = b/2</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,1/3</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 21' [210] at $3_21(1,1,2)1'$

**Asymmetric unit**

$0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq \frac{1}{6}$

**Vertices**

- $(0,0,0)$
- $(1,0,0)$
- $(1,1,0)$
- $(0,1,0)$
- $(0,0,\frac{1}{6})$
- $(1,0,\frac{1}{6})$
- $(1,1,\frac{1}{6})$
- $(0,1,\frac{1}{6})$

**Symmetry Operations**

**For 1 + set**

1. $1$
   - $(1|0,0,0)$

2. $3^*$
   - $(0,0,2/3)$
   - $(3z|0,0,2/3)$

3. $3'$
   - $(0,0,1/3)$
   - $(3z^-|0,0,1/3)$

4. $2$
   - $x,x,1/6$
   - $(2z|0,0,1/3)$

5. $2$
   - $x,2x,1/3$
   - $(2z|0,0,2/3)$

6. $2$
   - $2x,x,0$
   - $(2|0,0,0)$

**For 1' + set**

1. $1'$
   - $(1|0,0,0)'$

2. $3^*$
   - $(0,0,2/3)$
   - $(3z|0,0,2/3)'$

3. $3'$
   - $(0,0,1/3)$
   - $(3z^-|0,0,1/3)'$

4. $2'$
   - $x,x,1/6$
   - $(2z|0,0,1/3)'$

5. $2'$
   - $x,2x,1/3$
   - $(2z|0,0,2/3)'$

6. $2'$
   - $2x,x,0$
   - $(2|0,0,0)'$

153.2.1268 - 1 - 2725
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.  

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 11'</td>
<td>(1) x, y, z 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(2) y, x-y, z+2/3 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(3) x+y, x, z+1/3 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(4) y, x, z+1/3 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(5) x+y, y, z+2/3 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(6) x, x-y, z 0,0,0</td>
</tr>
<tr>
<td>3 b .21'</td>
<td>x, x, 1/6 0,0,0</td>
</tr>
<tr>
<td></td>
<td>x, 2x, 5/6 0,0,0</td>
</tr>
<tr>
<td></td>
<td>2x, x, 1/2 0,0,0</td>
</tr>
<tr>
<td>3 a .21'</td>
<td>x, x, 2/3 0,0,0</td>
</tr>
<tr>
<td></td>
<td>x, 2x, 1/3 0,0,0</td>
</tr>
<tr>
<td></td>
<td>2x, x, 0 0,0,0</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  
p3m11'  
a* = a   b* = b  
Origin at 0,0,z

Along [1,0,0]  
p1m11'  
a* = c   b* = (a+2b)/2  
Origin at x,0,1/3

Along [2,1,0]  
p2111'  
a* = c   b* = b/2  
Origin at x,x/2,0
Origin on 2' [210] at \(3_1(1,1,2')\)

Asymmetric unit: \(0 \leq x \leq 1; \ 0 \leq y \leq 1; \ 0 \leq z \leq 1/6\)

Vertices: 0,0,0, 1,0,0, 1,1,0, 0,1,0, 0,0,1/6, 1,0,1/6, 1,1,1/6, 0,1,1/6

Symmetry Operations:

1. \(1\)
2. \(3^* (0,0,2/3) \ 0,0,z\)
3. \(3^* (0,0,1/3) \ 0,0,z\)
4. \(2' \ x,x,1/6\)
5. \(2' \ x,2x,1/3\)
6. \(2' \ 2x,x,0\)

\( (1|0,0,0) \)
\( (3_z|0,0,2/3) \)
\( (3_z^-|0,0,1/3) \)
\( (2_z|0,0,1/3)' \)
\( (2_z|0,0,2/3)' \)
\( (2|0,0,0)' \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>c</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z+1/3 [v,u,w]</td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>x,x,1/6 [u,u,w]</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>x,x,2/3 [u,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections
Along [0,0,1]  p3m1
Along [1,0,0]  p1m1
Along [2,1,0]  p2'11
a* = a  b* = b
a* = c  b* = (a + 2b)/2
Origin at 0,0,z
Origin at x,0,1/3
Origin at x,x/2,0
Origin on 2 [210] at $3_21(1,1,2)$

Asymmetric unit: $0 \leq x < 1$; $0 \leq y < 1$; $0 \leq z < \frac{1}{6}$

Vertices:
- $0,0,0$
- $1,0,0$
- $1,1,0$
- $0,1,0$
- $0,0,\frac{1}{6}$
- $1,0,\frac{1}{6}$
- $1,1,\frac{1}{6}$
- $0,1,\frac{1}{6}$

Symmetry Operations

For $(0,0,0) +$ set

(1) $1$
(1) $0,0,0$
(2) $3^* (0,0,2/3)$
(3) $0,0,z$
(3) $3^* (0,0,1/3)$
(4) $0,0,2/3$
(2) $0,0,0$
(5) $2^* x,x,1/3$
(5) $2^* x,x,2/3$
(6) $2^* x,x,0$
(6) $2^* x,x,0$
(2) $0,0,1/3$'
(2) $0,0,0$'

For $(0,0,1) +$ set

(1) $t' (0,0,1)$
(1) $0,0,1$'
(2) $3^* (0,0,5/3)$
(3) $0,0,z$
(3) $3^* (0,0,4/3)$
(4) $0,0,5/3$'
(2) $0,0,1/3$'
(5) $2^* x,x,5/6$
(5) $2^* x,x,5/3$'
(6) $2^* x,x,1/2$
(6) $2^* x,x,1/2$
(2) $0,0,1$'

$P_{2c}\ 3_{2}12$  
$3121'$

Trigonal

$153.4.1270$  
$153.4.1270 - 1 - 2729$
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,-x-y,z+2/3 [v,u-v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+3/3 [u-v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z +1/3 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>b .2'</td>
<td>x,-x,1/6 [u,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,5/6 [u,0,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,1/2 [0,u,w]</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>a .2</td>
<td>x,-x,2/3 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,1/3 [u,2u,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,0 [2u,u,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p3m11'
- Along [1,0,0] p2_1 1m1
- Along [2,1,0] p2_1 211

<table>
<thead>
<tr>
<th>a* = a</th>
<th>b* = b</th>
<th>Origin at 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
<td>Origin at x,0,5/6</td>
</tr>
<tr>
<td>a* = c</td>
<td>b* = b/2</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin on 2 [110] at 3_2(1, 1, 2) 1

Asymmetric unit:

- Vertices:
  - 0, 0, 0
  - 1, 0, 0
  - 0, 0, 1/6
  - 1, 0, 1/6
  - 1, 1, 0
  - 0, 1, 0
  - 1, 1, 1/6
  - 0, 1, 1/6

Symmetry Operations:

1. $\mathbf{1}$
2. $3^*$ (0, 0, 2/3)
3. $3^*$ (0, 0, 1/3)
4. 2x, x, 0
5. 2x, x, 0, 1/6
6. 2x, x, 0, 2/3
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>c 1</td>
<td>(1) x,y,z [u,v,w]  (2) y,x-y,z+2/3 [v,u-v,w]  (3) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]  (5) x-y,y,z+1/3 [u-v,v,w]  (6) x,x+y,z+2/3 [u,u+v,w]</td>
</tr>
<tr>
<td>3</td>
<td>b .2.</td>
<td>x,0,1/6 [u,0,0]  0,x,5/6 [0,u,0]  x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td>3</td>
<td>a .2.</td>
<td>x,0,2/3 [u,0,0]  0,x,1/3 [0,u,0]  x,x,0 [u,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p31m'  Along [1,0,0]  p211  Along [2,1,0]  p1m'1
a* = a  b* = b  a* = c  b* = (a + 2b)/2  a* = c  b* = b/2
Origin at 0,0,z  Origin at x,0,1/6  Origin at x,x/2,1/3
Origin on 21' [110] at 3_2(1,1,2) 11'

Asymmetric unit

Vertices

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1,0,0</th>
<th>1,1,0</th>
<th>0,1,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
<td>0,1,1/6</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

For 1 + set

(1) 1
(1 | 0,0,0)

(2) 3' (0,0,2/3) 0,0,z
(3) 3' (0,0,1/3) 0,0,z
(4) 2' x,x,0
(5) 2' x,0,1/6
(6) 2' 0,y,1/3

(2_{xy} | 0,0,0)

(2_{xy} | 0,0,1/3)
(2_{y} | 0,0,2/3)

For 1' + set

(1) 1'
(1 | 0,0,0)'

(2) 3' (0,0,2/3) 0,0,z
(3) 3' (0,0,1/3) 0,0,z
(4) 2' x,x,0
(5) 2' x,0,1/6
(6) 2' 0,y,1/3

(2_{xy} | 0,0,0)'

(2_{xy} | 0,0,1/3)'
(2_{y} | 0,0,2/3)'

154.2.1272 - 1 - 2733
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>c</td>
<td>11'</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,y,z [0,0,0]</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>y,x-y,z+2/3 [0,0,0]</td>
<td>(2) y,x-y,z+2/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x+y,z+1/3 [0,0,0]</td>
<td>(3) x+y,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>.2.1'</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,0,1/6 [0,0,0]</td>
<td>(4) x,0,1/6 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,x,5/6 [0,0,0]</td>
<td>(5) x,0,5/6 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,1/2 [0,0,0]</td>
<td>(6) x,x,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m1'  
\[a^* = a \quad b^* = b\]
Origin at 0,0,z  
Along [1,0,0] p2111'  
\[a^* = c \quad b^* = (a + 2b)/2\]
Origin at x,0,1/6  
Along [2,1,0] p1m11'  
\[a^* = c \quad b^* = b/2\]
Origin at x,x/2,1/3
Origin on 2' [110] at 3\(_{3}(1,1,2')\) 1

Asymmetric unit

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0 ≤ x ≤ 1;</th>
<th>0 ≤ y ≤ 1;</th>
<th>0 ≤ z ≤ 1/6</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
<td>0,1,0</td>
</tr>
<tr>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
<td>0,1,1/6</td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 3' (0,0,2/3) 0,0,z
(3z | 0,0,2/3)

(3) 3' (0,0,1/3) 0,0,z
(3z⁻¹ | 0,0,1/3)

(4) 2' x,x,0
(2\(x\) | 0,0,0)'

(5) 2' x,0,1/6
(2\(x\) | 0,0,1/3)'

(6) 2' 0,y,1/3
(2\(y\) | 0,0,2/3)'

P3\(_2\) 2'1
154.3.1273
P3\(_2\) 2'1
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z+2/3 [v-u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
<td>(5) x-y,y,z+1/3 [u+v,v,w]</td>
</tr>
<tr>
<td>3 b .2'</td>
<td>x,0,1/6 [u,2u,w]</td>
<td>0,x,5/6 [2u,2u,w]</td>
</tr>
<tr>
<td>3 a .2'</td>
<td>x,0,2/3 [u,2u,w]</td>
<td>0,x,1/3 [2u,2u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2'11
\[ \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \]
Origin at x,0,1/6

Along [2,1,0] p1m1
\[ \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \]
Origin at x,x/2,1/3
Origin on 2 [110] at 3/1,1,2 1

Asymmetric unit 0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/6

Vertices
0,0,0 1,0,0 1,1,0 0,1,0
0,0,1/6 1,0,1/6 1,1,1/6 0,1,1/6

Symmetry Operations

For (0,0,0) + set

1 (1 0,0,0)
3* (0,0,2/3) 0,0,z
3* (0,0,1/3) 0,0,z
2 x,x,0 (2xy 0,0,0)
2* x,0,1/6 (2y,0,0,1/3)
2' 0,y,1/3 (2y,0,1/2)

For (0,0,1)' + set

1' (0,0,1)
3* (0,0,5/3) 0,0,z
3 (0,0,4/3) 0,0,z
2' x,x,1/2 (2xy 0,0,1/2)
2 x,0,2/3 (2x,0,0,3/2)
2 0,y,5/6 (2y,0,5/6)
Generators selected \( (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4). \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>c</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>6</td>
<td>a</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z ([u,v,w])</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>(2) (\bar{y},x-y,z+2/3 [\bar{v},u-v,w])</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>(3) (x+y,x,z+1/3 [u-v,u,w])</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>(4) (y,x,\bar{z} [v,u,\bar{w}])</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>(5) (x-y,y,z+1/3 [u+v,v,w])</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>(6) (x+y,z+2/3 [u,u+v,w])</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>p31m1'</th>
<th>Along [1,0,0]</th>
<th>p_{2c'}; 211</th>
<th>Along [2,1,0]</th>
<th>p_{2c';1m1}</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a \quad b^* = b)</td>
<td>(a^* = a \quad b^* = (a + 2b)/2)</td>
<td>(a^* = a \quad b^* = (a + 2b)/2)</td>
<td>(a^* = a \quad b^* = (a + 2b)/2)</td>
<td>(a^* = a \quad b^* = (a + 2b)/2)</td>
<td>(a^* = a \quad b^* = (a + 2b)/2)</td>
<td>(a^* = a \quad b^* = (a + 2b)/2)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,2/3</td>
<td>Origin at x,0,2/3</td>
<td>Origin at x,0,2/3</td>
<td>Origin at x,0,2/3</td>
<td>Origin at x,0,2/3</td>
<td>Origin at x,0,2/3</td>
</tr>
</tbody>
</table>
Origin on 32

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/6 & \quad 1/2,0,1/6 & \quad 2/3,1/3,1/6 & \quad 1/3,2/3,1/6 & \quad 0,1/2,1/6
\end{align*}
\]
Symmetry Operations

For (0,0,0) + set

(1) 1 (2) 3 0,0,z (3) 3 0,0,z
(1,0,0) (3; 0,0,0) (3; 0,0,0)

(4) 2 x,0,0 (5) 2 x,0,0 (6) 2 0,y,0
(2;x;0,0,0) (2;x;0,0,0) (2;y;0,0,0)

For (2/3,1/3,1/3) + set

(1) t (2/3,1/3,1/3) (2) 3* (0,0,1/3) 1/3,1/3,z
(1/2,3,1/3,1/3) (3; 2/3,1/3,1/3) (3; 0,0,1/3) 1/3,0,0,z

(4) 2 (1/2,1/2,0) x,x-1/6,1/6 (5) 2 (1/2,0,0) x,1/6,1/6
(2;x;2/3,1/3,1/3) (2;x;2/3,1/3,1/3)

For (1/3,2/3,2/3) + set

(1) t (1/3,2/3,2/3) (2) 3* (0,0,2/3) 0,1/3,z
(1/3,2/3,2/3) (3; 1/3,2/3,2/3) (3; 0,0,2/3) 1/3,1/3,z

(4) 2 (1/2,1/2,0) x,x+1/6,1/3 (5) 2 x,1/3,1/3
(2;x;1/3,2/3,2/3) (2;x;1/3,2/3,2/3)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 f 1</td>
<td>(0,0,0) +</td>
<td>(2/3,1/3,1/3) +</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>9 e .2</td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td>9 d .2</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
<td>6 c 3..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>3 b 32.</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>3 a 32.</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p3m'1

a* = (2a + b)/3 b* = (a + b)/3

Origin at 0,0,z

Along [1,0,0] p211

a* = (-a - 2b + c)/3 b* = (a + 2b)/2

Origin at x,0,0

Along [2,1,0] p1m'1

a* = c/3 b* = b/2

Origin at x,x/2,0
R321'  321'  Trigonal
155.2.1276  R321'
Origin on 321'

Asymmetric unit: \( 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \)

Vertices:
- \((0,0,0)\)
- \((2/3,1/3,0)\)
- \((1/3,2/3,0)\)
- \((0,1/2,0)\)
- \((0,0,1/6)\)
- \((1/2,0,1/6)\)
- \((2/3,1/3,1/6)\)
- \((1/3,2/3,1/6)\)
- \((0,1/2,1/6)\)
Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0) (2) \( 3^\prime \) 0,0,z (3) \( 3^\prime \) 0,0,z
(3_z | 0,0,0) (3_z | 0,0,0)

(4) 2 x,x,0
(2_x | 0,0,0) (5) 2 x,0,0 (6) 2 0,y,0
(2_x | 0,0,0) (2_y | 0,0,0)

For (2/3,1/3,1/3) + set

(1) t (2/3,1/3,1/3) (2) \( 3^\prime \) (0,0,1/3) 1/3,1/3,z (3) \( 3^\prime \) (0,0,1/3) 1/3,0,z
(1 | 2/3,1/3,1/3) (3_z | 2/3,1/3,1/3) (3_z | 2/3,1/3,1/3)

(4) 2 (1/2,1/2,0) x,x-1/6,1/6 (5) 2 (1/2,0,0) x,1/6,1/6 (6) 2 1/3,y,1/6
(2_x | 2/3,1/3,1/3) (2_x | 2/3,1/3,1/3) (2_y | 2/3,1/3,1/3)

For (1/3,2/3,2/3) + set

(1) t (1/3,2/3,2/3) (2) \( 3^\prime \) (0,0,2/3) 0,1/3,z (3) \( 3^\prime \) (0,0,2/3) 1/3,1/3,z
(1 | 1/3,2/3,2/3) (3_z | 1/3,2/3,2/3) (3_z | 1/3,2/3,2/3)

(4) 2 (1/2,1/2,0) x,x+1/6,1/3 (5) 2 x,1/3,1/3 (6) 2 (0,1/2,0) 1/6,y,1/3
(2_x | 1/3,2/3,2/3) (2_x | 1/3,2/3,2/3) (2_y | 1/3,2/3,2/3)

For (0,0,0)' + set

(1) 1'
(1 | 0,0,0)' (2) \( 3^\prime \) ' 0,0,z (3) \( 3^\prime \) ' 0,0,z
(3_z | 0,0,0)' (3_z | 0,0,0)'

(4) 2' x,x,0
(2_x | 0,0,0)' (5) 2' x,0,0 (6) 2' 0,y,0
(2_x | 0,0,0)' (2_y | 0,0,0)'

For (2/3,1/3,1/3)' + set

(1) t' (2/3,1/3,1/3) (2) \( 3^\prime \) ' (0,0,1/3) 1/3,1/3,z (3) \( 3^\prime \) ' (0,0,1/3) 1/3,0,z
(1 | 2/3,1/3,1/3)' (3_z | 2/3,1/3,1/3)' (3_z | 2/3,1/3,1/3)'

(4) 2' (1/2,1/2,0) x,x-1/6,1/6 (5) 2' (1/2,0,0) x,1/6,1/6 (6) 2' 1/3,y,1/6
(2_x | 2/3,1/3,1/3)' (2_x | 2/3,1/3,1/3)' (2_y | 2/3,1/3,1/3)'

For (1/3,2/3,2/3)' + set

(1) t' (1/3,2/3,2/3) (2) \( 3^\prime \) ' (0,0,2/3) 0,1/3,z (3) \( 3^\prime \) ' (0,0,2/3) 1/3,1/3,z
(1 | 1/3,2/3,2/3)' (3_z | 1/3,2/3,2/3)' (3_z | 1/3,2/3,2/3)'

(4) 2' (1/2,1/2,0) x,x+1/6,1/3 (5) 2' x,1/3,1/3 (6) 2' (0,1/2,0) 1/6,y,1/3
(2_x | 1/3,2/3,2/3)' (2_x | 1/3,2/3,2/3)' (2_y | 1/3,2/3,2/3)'

Generators selected (1): t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3);(2); (4): 1'.

155.2.1276 - 3 - 2744
Continued

155.2.1276
R321'

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>f</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,-x-y,z [0,0,0]</td>
<td>(2/3,1/3,1/3) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [0,0,0]</td>
<td>(1/3,2/3,2/3) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
<td>(0,0,0)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x-y,y,z [0,0,0]</td>
<td>(2/3,1/3,1/3) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x+y,z [0,0,0]</td>
<td>(1/3,2/3,2/3) +</td>
</tr>
<tr>
<td>9</td>
<td>e</td>
<td>(1) x,0,1/2 [0,0,0]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) 0,x,1/2 [0,0,0]</td>
<td>(2/3,1/3,1/3) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x,x,1/2 [0,0,0]</td>
<td>(1/3,2/3,2/3) +</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>(1) 0,0,z [0,0,0]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) 0,0,1/2 [0,0,0]</td>
<td>(2/3,1/3,1/3) +</td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>(1) 0,0,1/2 [0,0,0]</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>(1) 0,0,0 [0,0,0]</td>
<td>(0,0,0) +</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p3m1

\[ a^* = (2a + b)/3 \]
\[ b^* = (-a + b)/3 \]

Origin at 0,0,0

Along [1,0,0] p211

\[ a^* = (-a - 2b + c)/3 \]
\[ b^* = (a + 2b)/2 \]

Origin at x,0,0

Along [2,1,0] p1m1

\[ a^* = c/3 \]
\[ b^* = b/2 \]

Origin at x,x/2,0
Origin on 32'  

Asymmetric unit  
\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \]  

Vertices  
\begin{align*} 
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/6 & \quad 1/2,0,1/6 & \quad 2/3,1/3,1/6 & \quad 1/3,2/3,1/6 & \quad 0,1/2,1/6 
\end{align*}
Symmetry Operations

For \((0,0,0)\) + set

1. 1
2. 3' \(0,0,z\) (3) 3' \(0,0,z\)
   \((1,0,0)\) \((3z,0,0,0)\) \((3z,0,0,0)\)

4. 2' \(x,x,0\)
   \((2xy,0,0,0)\)
   \((2z,0,0,0)\)
   \((2y,0,0,0)\)

For \((2/3,1/3,1/3)\) + set

1. \(t(2/3,1/3,1/3)\)
   \((1,0,0)\)
   \((2z,2/3,1/3,1/3)\)
   \((3z,1/3,1/3,1/3)\)

4. 2' \((1/2,1/2,0)\)
   \((2xy,2/3,1/3,1/3)\)
   \((2z,2/3,1/3,1/3)\)
   \((2y,2/3,1/3,1/3)\)

For \((1/3,2/3,2/3)\) + set

1. \(t(1/3,2/3,2/3)\)
   \((1,0,0)\)
   \((2z,1/3,2/3,2/3)\)
   \((3z,1/3,2/3,2/3)\)

4. 2' \((1/2,1/2,0)\)
   \((2xy,1/3,2/3,2/3)\)
   \((2z,1/3,2/3,2/3)\)
   \((2y,1/3,2/3,2/3)\)

Generators selected

\((1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).\)

Positions

- Multiplicity
- Wyckoff letter
- Site Symmetry
- Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>f</td>
<td>((0,0,0)) + ((2/3,1/3,1/3)) + ((1/3,2/3,2/3))</td>
<td></td>
</tr>
<tr>
<td>9 e (2')</td>
<td>x,0,1/2 ([u,2u,w])</td>
<td>(0,x,1/2 ([2u,\bar{u},w])</td>
<td>(\bar{x},x,1/2 ([u,u,w])</td>
</tr>
<tr>
<td>9 d (2')</td>
<td>x,0,0 ([u,2u,w])</td>
<td>(0,x,0 ([2u,\bar{u},w])</td>
<td>(\bar{x},x,0 ([u,u,w])</td>
</tr>
<tr>
<td>6 c (3')</td>
<td>0,0,0 ([0,0,w])</td>
<td>0,0,0 ([0,0,w])</td>
<td></td>
</tr>
<tr>
<td>3 b (32')</td>
<td>0,0,1/2 ([0,0,w])</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 a (32')</td>
<td>0,0,0 ([0,0,w])</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along \([0,0,1]\) \(p3m1\)
  \(a^* = (2a + b)/3\) \(b^* = (-a + b)/3\) \(a^* = (-a - 2b + c)/3\) \(b^* = (a + 2b)/2\)
  Origin at \(0,0,z\)

- Along \([1,0,0]\) \(p2'11\)
  \(a^* = (-a - 2b + c)/3\) \(b^* = (a + 2b)/2\)
  Origin at \(x,0,0\)

- Along \([2,1,0]\) \(p1m1\)
  \(a^* = c/3\) \(b^* = b/2\)
  Origin at \(x,x/2,0\)
Origin on 32

Asymmetric unit: $0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$

Vertices:
- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/6$
- $1/2,0,1/6$
- $2/3,1/3,1/6$
- $1/3,2/3,1/6$
- $0,1/2,1/6$
Symmetry Operations

For (0,0,0) + set

1 1 0,0,0
(1) 1 (2) 3 0,0,z
(3) 3 0,0,z
(1) (2,0,0,0) (2,0,0,0) (2,0,0,0)
(3) (2,0,0,0) (2,0,0,0) (2,0,0,0)
(4) 2 x,x,0 (5) 2 x,0,0
(6) 2 y,0,0
(2,x) (2,x) (2,x)
For (2/3,1/3,1/3)' + set

1 1/2,1/3,1/3
(1) t 2/3,1/3,1/3 (2) 3 0,0,1/3
(3) 3 0,0,1/3 (3) 3 0,0,1/3 (3) 3 0,0,1/3
(1) (2,0,0,0) (2,0,0,0) (2,0,0,0) (2,0,0,0)
For (1/3,2/3,2/3) + set

1 1/2,1/3,1/3
(1) t 1/3,2/3,2/3 (2) 3 0,0,2/3
(3) 3 0,0,1/3 (3) 3 0,0,1/3 (3) 3 0,0,1/3
(1) (2,0,0,0) (2,0,0,0) (2,0,0,0) (2,0,0,0)

Generators selected

1; t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3);(2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td>9</td>
<td>(2/3,1,3/3)' +</td>
</tr>
<tr>
<td>6</td>
<td>(1/3,2/3,2/3) +</td>
</tr>
</tbody>
</table>

18 f 1
(1) x,y,z [u,v,w] (2) y,x-y,z [v.u-w] (3) x+y,x,x [u+v,u+w]
(4) y,x,z [v.u,w] (5) x-y,y,z [u-v,v+w] (6) x,x+y,z [u+v,u+w]
9 e .2'
(7) x,0,1/2 [u,2u,w] (8) 0,x,1/2 [2u,u,w] x,x,1/2 [u,u,w]
9 d .2
9 e .2
3 c 3..
3 b 32'
3 a 32

Symmetry of Special Projections

Along [0,0,1] p3m11' a* = (2a + b)/3 b* = (-a + b)/3 Origin at 0,0,z
Along [1,0,0] p3211 a* = (-a - 2b + c)/3 b* = (a + 2b)/2 Origin at x,0,0
Along [2,1,0] p6m1 a* = c/3 b* = b/2 Origin at x,x/2,0

Along [2,1,0] p3211 a* = (2a + b)/3 b* = (-a + b)/3 Origin at 0,0,z
Along [1,0,0] p3211 a* = (-a - 2b + c)/3 b* = (a + 2b)/2 Origin at x,0,0
Along [2,1,0] p6m1 a* = c/3 b* = b/2 Origin at x,x/2,0
**Origin** on 3m1

**Asymmetric unit**

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq 1; \quad x \leq 2y; \quad y \leq \min(1-x,2x) \]

**Vertices**

- 0,0,0
- 2/3,1/3,0
- 1/3,2/3,0
- 0,0,1
- 2/3,1/3,1
- 1/3,2/3,1

**Symmetry Operations**

1. \[1\]
   - \([1\mid 0,0,0]\)

2. \[3^+\]
   - \([0,0,z]\)
   - \([3_z\mid 0,0,0]\)

3. \[3\]
   - \([0,0,z]\)
   - \([3_z^{-1}\mid 0,0,0]\)

4. \[m\]
   - \(x, x, z\)
   - \([m_{xy}\mid 0,0,0]\)

5. \[m\]
   - \(x, 2x, z\)
   - \([m_x\mid 0,0,0]\)

6. \[m\]
   - \(2x, x, z\)
   - \([m_y\mid 0,0,0]\)
**Generators selected**  
\(1\); \(t(1,0,0); t(0,1,0); t(0,0,1); \) \((2); (4)\).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| \(6\) | e | 1 | \((1)\) \(x,y,z\) \([u,v,w]\)  
\((2)\) \(y , x-y,z\) \([v , u-v,w]\)  
\((3)\) \(x+y,x ,z\) \([u+v,u,w]\)  
\((4)\) \(y , x,z\) \([v,u,w]\)  
\((5)\) \(x+y,y,z\) \([u-v,v,w]\)  
\((6)\) \(y , x,z\) \([v,u,w]\) |
| \(3\) | d | .m. | \(x,x,z\) \([u,u,0]\)  
\(x,2x,z\) \([u,0,0]\)  
\(2x,x,z\) \([0,u,0]\) |
| \(1\) | c | 3m. | \(2/3,1/3,z\) \([0,0,0]\) |
| \(1\) | b | 3m. | \(1/3,2/3,z\) \([0,0,0]\) |
| \(1\) | a | 3m. | \(0,0,z\) \([0,0,0]\) |

**Symmetry of Special Projections**

- Along \([0,0,1]\) p3m1  
- Along \([1,0,0]\) \(p11^*\)  
- Along \([2,1,0]\) p1m1

\(a^* = a\)  
\(b^* = b\)  
\(a^* = c\)  
\(b^* = (a + 2b)/2\)  
\(a^* = b/2\)  
\(b^* = c\)  

Origin at \(0,0,z\)  
Origin at \(x,0,0\)  
Origin at \(x,x/2,0\)
Origin on 3m11' denotes the origin is on the 3m11' plane.

Asymmetric unit:

- 0 ≤ x ≤ 2/3;
- 0 ≤ y ≤ 2/3;
- 0 ≤ z ≤ 1;
- x < 2y;
- y ≤ min(1-x, 2x)

Vertices:

- 0,0,0
- 2/3,1/3,0
- 1/3,2/3,0
- 0,0,1
- 2/3,1/3,1
- 1/3,2/3,1

Symmetry Operations:

For 1 + set:

1. 1
2. 3* 0,0,z
3. 3' 0,0,z
4. m x,x,z
   (m_{xy}|0,0,0)
5. m x,2x,z
   (m_{x}|0,0,0)
6. m 2x,x,z
   (m_{y}|0,0,0)

For 1' + set:

1'. 1'
2. 3*' 0,0,z
3. 3' 0,0,z
4. m' x,x,z
   (m_{xy}|0,0,0)
5. m' x,2x,z
   (m_{x}|0,0,0)
6. m' 2x,x,z
   (m_{y}|0,0,0)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 e 11' x,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>3 d .m.1' x,x,z [0,0,0]</td>
<td>x,2x,z [0,0,0]</td>
</tr>
<tr>
<td>1 c 3m.1' 2/3,1/3,z [0,0,0]</td>
<td>2x,x,z [0,0,0]</td>
</tr>
<tr>
<td>1 b 3m.1' 1/3,2/3,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a 3m.1' 0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1] p3m11'**
  - \(a^* = a\) \(b^* = b\)
  - Origin at 0,0,z

- **Along [1,0,0] p11'**
  - \(a^* = c\) \(b^* = (a + 2b)/2\)
  - Origin at x,0,0

- **Along [2,1,0] p1m11'**
  - \(a^* = b/2\) \(b^* = c\)
  - Origin at x,x/2,0
Origin on 3m'1

Asymmetric unit:

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; 0 ≤ z ≤ 1; x ≤ 2y; y ≤ min(1-x,2x)

Vertices:

0,0,0 2/3,1/3,0 1/3,2/3,0
0,0,1 2/3,1/3,1 1/3,2/3,1

Symmetry Operations:

(1) 1
   (1 | 0,0,0)

(2) 3
   (0,0,2x)
   (0,0,0)
(3) 3
   (0,0,0)
   (0,0,0)
(3) 3
   (0,0,0)
   (0,0,0)
(4) m' x,x,z
   (m,0,0,0)
(5) m' x,2x,z
   (m,0,0,0)
(6) m' 2x,x,z
   (m,0,0,0)
   (m,0,0,0)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>6 e 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>3 d .m'</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>1 c 3m'</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>1 b 3m'</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>1 a 3m'</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p3m'1</th>
<th>Along [1,0,0]</th>
<th>p1</th>
<th>Along [2,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>a</strong> = a, <strong>b</strong> = b</td>
<td><strong>a</strong> = a, <strong>b</strong> = b</td>
<td><strong>a</strong> = c, <strong>b</strong> = (a + 2b)/2</td>
<td><strong>a</strong> = b/2, <strong>b</strong> = c</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on 3m1

Asymmetric unit

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 &lt; x &lt; 2/3;</td>
<td>0 &lt; y &lt; 2/3;</td>
<td>0 &lt; z &lt; 1;</td>
</tr>
<tr>
<td>x &lt; 2y;</td>
<td>y &lt; min(1-x,2x)</td>
<td></td>
</tr>
</tbody>
</table>

Vertices

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>2/3,1/3,0</td>
<td>1/3,2/3,0</td>
</tr>
<tr>
<td>0,0,1</td>
<td>2/3,1/3,1</td>
<td>1/3,2/3,1</td>
</tr>
</tbody>
</table>

Symmetry Operations

For (0,0,0) + set

1. 1
   (1)\(1\) 0,0,0

2. 3\(\ast\) 0,0,z
   (2) 3\(\ast\) 0,0,z
   \(3\) 3\(\ast\) 0,0,z

3. m\(\times\) ,x,z
   (4) m\(\times\) ,x,z
   \(m\)\(\times\) 0,0,0

4. c\(\times\) (0,0,1)
   (5) c\(\times\) (0,0,1)
   \(c\)\(\times\) 0,0,0

5. c\(\times\) (0,0,1)\(\ast\)
   (6) c\(\times\) (0,0,1)\(\ast\)
   \(c\)\(\times\) 0,0,0

For (0,0,1)\(\ast\) + set

1. t\(\ast\) (0,0,1)
   (1) t\(\ast\) (0,0,1)\(\ast\)

2. 3\(\ast\) \(\ast\) (0,0,1) 0,0,z
   (2) 3\(\ast\) \(\ast\) (0,0,1) 0,0,z
   \(3\) 3\(\ast\) \(\ast\) (0,0,1) 0,0,z

3. m\(\times\) ,x,z
   (4) m\(\times\) ,x,z
   \(m\)\(\times\) 0,0,0

4. c\(\times\) (0,0,1)\(\ast\)
   (5) c\(\times\) (0,0,1)\(\ast\)
   \(c\)\(\times\) 0,0,0

5. c\(\times\) (0,0,1)\(\ast\)
   (6) c\(\times\) (0,0,1)\(\ast\)
   \(c\)\(\times\) 0,0,0

156.4.1282 - 1 - 2758
Generators selected: (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

**Positions**

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<tr>
<th>Multiplicity</th>
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<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>12</td>
<td>e</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x+y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x-y,z [u,u+v,w]</td>
</tr>
<tr>
<td>6</td>
<td>d</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] p3m11'
  - a* = a  \(b^* = b\)
  - Origin at 0,0,z

- Along [1,0,0] p11'
  - a* = c  \(b^* = (a + 2b)/2\)
  - Origin at x,0,0

- Along [2,1,0] p2\(\gamma\) 1m1
  - a* = b/2  \(b^* = c\)
  - Origin at x,x/2,0
Origin on 3m'1

Asymmetric unit

\[0 < x < \frac{2}{3}; \quad 0 < y < \frac{2}{3}; \quad 0 < z < 1; \quad x < 2y; \quad y \leq \min(1-x,2x)\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 \\
0,0,1 & \quad 2/3,1/3,1 & \quad 1/3,2/3,1
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(1'0,0,0) & \quad (2) 3' \quad 0,0,z \\
& \quad (3_z'0,0,0) \\
& \quad (3_z'0,0,0') \\
(4) m' \quad x,x,z & \quad (5) m' \quad x,2x,z \\
(m_{xy}|0,0,0)' & \quad (m_{xy}|0,0,0)'
\end{align*}
\]

For \((0,0,1) + \) set

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(1'0,0,1) & \quad (2) 3' \quad (0,0,1) \quad 0,0,z \\
& \quad (3_z|0,0,1) \\
& \quad (3_z|0,0,1') \\
(4) c \quad (0,0,1) \quad x,x,z & \quad (5) c \quad (0,0,1) \quad x,2x,z \\
(m_{xy}|0,0,1) & \quad (m_{xy}|0,0,1) \\
& \quad (m_{xy}|0,0,1)'
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

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</tr>
<tr>
<td></td>
<td>(2) y, x-y, z [v, u-v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) x+y, x, z [u+v, u, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) y', x, z [v, u, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) x+y, y, z [u+v, v, w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(6) x-y, x, z [u-v, v, w]</td>
<td></td>
</tr>
</tbody>
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<table>
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<tr>
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</thead>
<tbody>
<tr>
<td>Along [0, 0, 1] p3m11'</td>
</tr>
<tr>
<td>a* = a  b* = b</td>
</tr>
<tr>
<td>Origin at 0, 0, z</td>
</tr>
</tbody>
</table>
**Origin** on 31m

**Asymmetric unit**  
0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1;  
x ≤ (1+y)/2;  y ≤ min(1-x,x)

**Vertices**  
0,0,0  1/2,0,0  2/3,1/3,0  1/2,1/2,0  1/2,1/2,1

0,0,1  1/2,0,1  2/3,1/3,1  1/2,1/2,1

**Symmetry Operations**

(1) 1  
(1|0,0,0)

(2) $3^*$ 0,0,z  
(3z$^*$|0,0,0)

(3) $3'$ 0,0,z  
(3z$^{-1}$|0,0,0)

(4) m x,x,z  
(m$|_3$|0,0,0)

(5) m x,0,z  
(m$|_2$|0,0,0)

(6) m 0,y,z  
(m$_1$|0,0,0)
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

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<td>d</td>
<td>1 (1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x-y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x+y,z [u,u-v,w]</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>0,x,z [2u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,z [u,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p31m</th>
<th>Along [1,0,0]</th>
<th>p1m1</th>
<th>Along [2,1,0]</th>
<th>p11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (a + 2b)/2</td>
<td>b* = c</td>
<td>a* = c</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 31m1'

Asymmetric unit

- $0 \leq x \leq 2/3$;
- $0 \leq y \leq 1/2$;
- $0 \leq z \leq 1$;
- $x \leq (1+y)/2$;
- $y \leq \min(1-x,x)$

Vertices

- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/2,1/2,0$
- $0,0,1$
- $1/2,0,1$
- $2/3,1/3,1$
- $1/2,1/2,1$

Symmetry Operations

For 1 + set

1. $1$
   - $(1 | 0,0,0)$

2. $3 \cdot 0,0,z$
   - $(3_z | 0,0,0)$

3. $3 \cdot 0,0,z$
   - $(3_z^{-1} | 0,0,0)$

4. $m \cdot x,z$
   - $(m_3 | 0,0,0)$

5. $m \cdot x,0,z$
   - $(m_2 | 0,0,0)$

6. $m \cdot 0,y,z$
   - $(m_1 | 0,0,0)$

For 1' + set

1'. $1'$
   - $(1 | 0,0,0)'$

2'. $3 \cdot 0,0,z$
   - $(3_z | 0,0,0)'$

3'. $3 \cdot 0,0,z$
   - $(3_z^{-1} | 0,0,0)'$

4'. $m' \cdot x,z$
   - $(m_3 | 0,0,0)'$

5'. $m' \cdot x,0,z$
   - $(m_2 | 0,0,0)'$

6'. $m' \cdot 0,y,z$
   - $(m_1 | 0,0,0)'$
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4): 1'. \)

**Positions**

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<tbody>
<tr>
<td>6</td>
<td>d</td>
<td>(1, x,y,z [0,0,0] )</td>
<td>1 +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2, \bar{y},x-y,z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3, \bar{x}+y,\bar{x},z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4, y,x,z [0,0,0] )</td>
<td>1' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5, x-y,y,z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6, x,x+y,z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>(x,0,z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(0,x,z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\bar{x},\bar{x},z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>(1/3,2/3,z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2/3,1/3,z [0,0,0] )</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>(0,0,z [0,0,0] )</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) \( \text{p31m1'} \)
  - \(a^* = a\)
  - \(b^* = b\)
- Origin at 0,0,z

- Along \([1,0,0]\) \( \text{p1m11'} \)
  - \(a^* = (a+2b)/2\)
  - \(b^* = c\)
- Origin at x,0,0

- Along \([2,1,0]\) \( \text{p11'} \)
  - \(a^* = c\)
  - \(b^* = b/2\)
- Origin at x,x/2,0
Origin on 31m'

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq \frac{2}{3}; & 0 \leq y & \leq \frac{1}{2}; & 0 \leq z & \leq 1; & x & \leq \frac{1+y}{2}; & y & \leq \min(1-x,x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1 & \quad 1/2,1/2,1
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^z \quad 0,0,z \\
(3) & \quad 3^{-1} \quad 0,0,z \\
(4) & \quad m' \quad x,x,z \\
(5) & \quad m' \quad x,0,z \\
(6) & \quad m' \quad 0,y,z
\end{align*}
\]

\[
\begin{align*}
(1) & \quad 1 \quad (0,0,0) \\
(2) & \quad 3^z \quad 0,0,0 \\
(3) & \quad 3^{-1} \quad 0,0,0 \\
(4) & \quad m' \quad (0,0,0)' \\
(5) & \quad m' \quad (0,0,0)' \\
(6) & \quad m' \quad (0,0,0)'
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td></td>
<td></td>
<td>(4) y,x,z [v,u,w] (5) x-y,y,z [u-v,v,w] (6) x,x+y,z [u,u+v,w]</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>.m' x,0,z [u,0,w] 0,x,z [0,u,w] x,x,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>3.. 1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>3..m' 0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m'  Along [1,0,0] p1m'1  Along [2,1,0] p1

\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \quad \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \quad \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)

Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
Origin on 31m

Asymmetric unit

\[ 0 < x < \frac{2}{3}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < 1; \quad x < \frac{1+y}{2}; \quad y \leq \min(1-x,x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1 & \quad 1/2,1/2,1
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(2) & \quad (3_z,0,0,0) \\
(3) & \quad 3' \quad 0,0,z \\
(3) & \quad (3_z^{-1},0,0,0) \\
(4) & \quad m \quad x,x,z \\
(4) & \quad (m_3|0,0,0) \\
(5) & \quad m \quad x,0,z \\
(5) & \quad (m_2|0,0,0) \\
(6) & \quad m \quad 0,y,z \\
(6) & \quad (m_1|0,0,0)
\end{align*}
\]

For \((0,0,1)' + \text{set}\)

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(1) & \quad (0,0,1)' \\
(2) & \quad 3' \quad (0,0,1) \quad 0,0,z \\
(2) & \quad (3_z,0,0,1)' \\
(3) & \quad 3' \quad (0,0,1) \quad 0,0,z \\
(3) & \quad (3_z^{-1},0,0,1)' \\
(4) & \quad c' \quad (0,0,1) \quad x,x,z \\
(4) & \quad (m_3|0,0,1)' \\
(5) & \quad c' \quad (0,0,1) \quad x,0,z \\
(5) & \quad (m_2|0,0,1)' \\
(6) & \quad c' \quad (0,0,1) \quad 0,y,z \\
(6) & \quad (m_1|0,0,1)'
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

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<tr>
<td>12</td>
<td>d</td>
<td>(0,0,0) + (0,0,1)' + (0,0,0)</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>x,0,z [u,2u,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Coordinates

| (1) x,y,z [u,v,w] | (2) y,z-x,y,z [v,u-v,w] | (3) x+u,y,z [u+v,u,w] |
| (4) y,x,z [v,u,w] | (5) x+y,z [u+v,v,w] | (6) x,y,z [u,u+v,w] |

Symmetry of Special Projections

- Along [0,0,1] p31m1'  
  \( a^* = a \) \( b^* = b \)  
  Origin at 0,0,z

- Along [1,0,0] p2b' 1m1  
  \( a^* = (a + 2b)/2 \) \( b^* = c \)  
  Origin at x,0,0

- Along [2,1,0] p11'  
  \( a^* = c \) \( b^* = b/2 \)  
  Origin at x,x/2,0
Origin on 31m'

Asymmetric unit:

\[ 0 < x < 2/3; \quad 0 < y < 1/2; \quad 0 < z < 1; \quad x < (1+y)/2; \quad y < \min(1-x,x) \]

Vertices:

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
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<th></th>
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<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
<td>1/2,1/2,0</td>
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<tr>
<td>0,0,1</td>
<td>1/2,0,1</td>
<td>2/3,1/3,1</td>
<td>1/2,1/2,1</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations:

For (0,0,0) + set:

(1) 1
(1) 0,0,0
(2) \(3^z\) 0,0,z
(3) \(3^{-1}\) 0,0,z
(4) \(m'\) x,x,z
(5) \(m'\) x,0,z
(6) \(m'\) 0,y,z
(7) \(m_1\) 0,0,0

For (0,0,1) + set:

(1) \(t'\) (0,0,1)
(1) (0,0,1)'
(2) \(3'\) (0,0,1) 0,0,z
(3) \(3'\) (0,0,1) 0,0,z
(4) \(c\) (0,0,1) x,x,z
(5) \(c\) (0,0,1) x,0,z
(6) \(c\) (0,0,1) 0,y,z
Generators selected: (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
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<td>c</td>
<td>x,0,z [u,0,w]</td>
</tr>
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<td>b</td>
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</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m1'   Along [1,0,0] p2a1 1m'1   Along [2,1,0] p2a1 1
\(a^* = a\) \(b^* = b\) \(a^* = (a + 2b)/2\) \(b^* = c\) \(a^* = c\) \(b^* = b/2\)
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
**Origin** on 3c1

**Asymmetric unit**

- $0 \leq x < 2/3;$
- $0 \leq y < 2/3;$
- $0 \leq z < 1/2;$
- $x < (1+y)/2;$
- $y \leq \min(1-x,(1+x)/2)$

**Vertices**

- $0,0,0$
- $0,0,1/2$
- $1/2,0,0$
- $1/2,0,1/2$
- $2/3,1/3,0$
- $2/3,1/3,1/2$
- $1/3,2/3,0$
- $1/3,2/3,1/2$
- $0,1/2,0$
- $0,1/2,1/2$

**Symmetry Operations**

1. $1$
   - $(1|0,0,0)$
2. $3^{+}$ $0,0,z$
   - $(3_{z}|0,0,0)$
3. $3^{-}$ $0,0,z$
   - $(3_{z}^{-1}|0,0,0)$
4. $c$ $(0,0,1/2)$ $x,x,z$
   - $(m_{y}|0,0,1/2)$
5. $c$ $(0,0,1/2)$ $x,2x,z$
   - $(m_{x}|0,0,1/2)$
6. $c$ $(0,0,1/2)$ $2x,x,z$
   - $(m_{y}|0,0,12)$
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4). \)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
</tbody>
</table>
| 6 d 1 | \( (1) x,y,z [u,v,w] \) \( (2) y,x-y,z [v,u-v,w] \) \( (3) x+y,x,z [u+v,u,w] \)
| | \( (4) y,x,z+1/2 [v,u,w] \) \( (5) x+y,y,z+1/2 [u-v,v,w] \) \( (6) x,x-y,z+1/2 [u,u+v,w] \) |
| 2 c 3.. | \( 2/3,1/3,z [0,0,w] \) \( 2/3,1/3,z+1/2 [0,0,w] \) |
| 2 b 3.. | \( 1/3,2/3,z [0,0,w] \) \( 1/3,2/3,z+1/2 [0,0,w] \) |
| 2 a 3.. | \( 0,0,z [0,0,w] \) \( 0,0,z+1/2 [0,0,w] \) |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p3m1</th>
<th>Along [1,0,0] p( \text{hex}^* ), 1</th>
<th>Along [2,1,0] p1g1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a \quad b^* = b )</td>
<td>( a^* = c/2 \quad b^* = (a + 2b)/2 )</td>
<td>( a^* = b/2 \quad b^* = c )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin on 3c11'

Asymmetric unit

\[
\begin{align*}
0 & \leq x \leq 2/3; & 0 & \leq y \leq 2/3; & 0 & \leq z \leq 1/2; & x & \leq (1+y)/2; & y & \leq \min(1-x,(1+x)/2) \\
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/3,2/3,0 & & 0,1/2,0 \\
0,0,1/2 & & 1/2,0,1/2 & & 2/3,1/3,1/2 & & 1/3,2/3,1/2 & & 0,1/2,1/2 \\
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^* \quad 0,0,z \\
(4) & \quad c \quad (0,0,1/2) \quad x,x,z \\
(5) & \quad c \quad (0,0,1/2) \quad x,2x,z \\
(6) & \quad c \quad (0,0,1/2) \quad 2x,x,z \\
\end{align*}
\]

For 1' + set

\[
\begin{align*}
(1) & \quad 1' \\
(2) & \quad 3^{*'} \quad 0,0,z \\
(3) & \quad 3^{*'} \quad 0,0,z \\
(4) & \quad c' \quad (0,0,1/2) \quad x,x,z \\
(5) & \quad c' \quad (0,0,1/2) \quad x,2x,z \\
(6) & \quad c' \quad (0,0,1/2) \quad 2x,x,z \\
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
<th>multiplicity</th>
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<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>d</td>
<td>1' x,y,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>3..1' 2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>3..1' 1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>3..1' 0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p3m11'  
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p11'  
\[ a^* = c/2 \quad b^* = (a + 2b)/2 \]
Origin at x,0,0

Along [2,1,0] p1g11'  
\[ a^* = b/2 \quad b^* = c \]
Origin at x,x/2,0
**Origin** on 3c'1

**Asymmetric unit**

- $0 \leq x < 2/3$
- $0 \leq y < 2/3$
- $0 \leq z < 1/2$
- $x \leq (1+y)/2$
- $y \leq \min(1-x,(1+x)/2)$

**Vertices**

- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/2$
- $1/2,0,1/2$
- $2/3,1/3,1/2$
- $1/3,2/3,1/2$
- $0,1/2,1/2$

**Symmetry Operations**

1. $1$
   - $(1 | 0,0,0)$
   - $(1 | 0,0,0)$
2. $3^*$
   - $0,0,z$
   - $(3_z | 0,0,0)$
3. $3^*$
   - $0,0,z$
   - $(3_z^{-1} | 0,0,0)$
4. $c'$
   - $(0,0,1/2)$
   - $x,x,z$
   - $(m_x | 0,0,1/2)'$
5. $c'$
   - $(0,0,1/2)$
   - $x,2x,z$
   - $(m_x | 0,0,1/2)'$
6. $c'$
   - $(0,0,1/2)$
   - $2x,x,z$
   - $(m_y | 0,0,12)'$

**P3c'1  3m'1  Trigonal**

158.3.1291  

P3c'1
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6  d  1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y, x-y,z [v, u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y, x, z [u+v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(4) y, x, z+1/2 [v, u, w]</td>
</tr>
<tr>
<td></td>
<td>(5) x+y, y, z+1/2 [u+v, v, w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y, y, z+1/2 [u, u-v, w]</td>
</tr>
<tr>
<td>2  c  3..</td>
<td>2/3, 1/3, z [0,0, w]</td>
</tr>
<tr>
<td></td>
<td>2/3, 1/3, z+1/2 [0,0, w]</td>
</tr>
<tr>
<td>2  b  3..</td>
<td>1/3, 2/3, z [0,0, w]</td>
</tr>
<tr>
<td></td>
<td>1/3, 2/3, z+1/2 [0,0, w]</td>
</tr>
<tr>
<td>2  a  3..</td>
<td>0,0, z [0,0, w]</td>
</tr>
<tr>
<td></td>
<td>0,0, z+1/2 [0,0, w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p3m'1  Along [1,0,0]  p1  Along [2,1,0]  p1g'1

\( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)  \( \mathbf{a}^* = \mathbf{c}/2 \)  \( \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)  \( \mathbf{a}^* = \mathbf{b}/2 \)  \( \mathbf{b}^* = \mathbf{c} \)

Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
**Origin** on 31c

**Asymmetric unit**

\[
\begin{align*}
0 & \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x, (1+x)/2)
\end{align*}
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2 & \quad 0,1/2,1/2
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 & \quad (2) & \quad 3^+ & \quad (3) & \quad 3^- \\
(1 | 0,0,0) & \quad (0,0,z) & \quad (0,0,0) & \quad (0,0,z) & \quad (0,0,0) \\
(4) & \quad c & \quad (0,0,1/2) & \quad x,x,z & \quad (5) & \quad c & \quad (0,0,1/2) & \quad x,0,z & \quad (6) & \quad c & \quad (0,0,1/2) & \quad 0,y,z & \quad (m,0,0,1/2)
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

**Positions**

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<tbody>
<tr>
<td>6</td>
<td>c</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x-y,y,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x+y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1]  p31m  Along [1,0,0]  p1g1  Along [2,1,0]  p2a1
a* = a  b* = b  a* = (a + 2b)/2  b* = c  a* = c/2  b* = b/2
Origin at 0,0,z  Origin at 0,0,0  Origin at x,x/2,0
Origin on 31c'

Asymmetric unit

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; 0 ≤ z ≤ 1/2; x ≤ (1+y)/2; y ≤ min(1-x,(1+x)/2)

Vertices

0,0,0 1/2,0,0 2/3,1/3,0 1/3,2/3,0 0,1/2,0 0,0,1/2 1/2,0,1/2 2/3,1/3,1/2 1/3,2/3,1/2 0,1/2,1/2

Symmetry Operations

For 1 + set

(1) 1
(1 | 0,0,0)

(2) 3' 0,0,z
(3'z | 0,0,0)

(4) c (0,0,1/2) x,x,z
(m_3 | 0,0,1/2)

(5) c (0,0,1/2) x,0,z
(m_2 | 0,0,1/2)

(6) c (0,0,1/2) 0,y,z
(m_1 | 0,0,1/2)

For 1' + set

(1) 1'
(1 | 0,0,0)'

(2) 3' 0,0,z
(3'z | 0,0,0)'

(4) c' (0,0,1/2) x,x,z
(m_3 | 0,0,1/2)'

(5) c' (0,0,1/2) x,0,z
(m_2 | 0,0,1/2)'

(6) c' (0,0,1/2) 0,y,z
(m_1 | 0,0,1/2)'

159.2.1293 - 1 - 2780
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

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<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x-y,y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x+y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
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<td>a</td>
<td>0,0,z [0,0,0]</td>
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</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p31m1'</th>
<th>Along [1,0,0]</th>
<th>p1g11'</th>
<th>Along [2,1,0]</th>
<th>p11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (a + 2b)/2</td>
<td>b* = c</td>
<td>a* = c/2</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on 31c'

**Asymmetric unit**

- $0 < x < \frac{2}{3}$; $0 < y < \frac{2}{3}$; $0 < z < \frac{1}{2}$; $x < \frac{1+y}{2}$; $y \leq \min(1-x,(1+x)/2)$

**Vertices**

- $0,0,0$
- $0,0,\frac{1}{2}$
- $\frac{1}{2},0,0$
- $\frac{1}{2},0,\frac{1}{2}$
- $\frac{2}{3},\frac{1}{3},0$
- $\frac{2}{3},\frac{1}{3},\frac{1}{2}$
- $\frac{1}{3},\frac{2}{3},0$
- $\frac{1}{3},\frac{2}{3},\frac{1}{2}$
- $0,\frac{1}{2},0$
- $0,\frac{1}{2},\frac{1}{2}$
- $\frac{1}{2},\frac{1}{2},0$
- $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

**Symmetry Operations**

1. $1$
   
   $(1 | 0,0,0)$

2. $3^+ 0,0,z$
   
   $(3_z | 0,0,0)$

3. $3^- 0,0,z$
   
   $(3_z^{-1} | 0,0,0)$

4. $c' (0,0,1/2) x,x,z$
   
   $(m_{3} | 0,0,1/2)'$

5. $c' (0,0,1/2) x,0,z$
   
   $(m_{2} | 0,0,1/2)'$

6. $c' (0,0,1/2) 0,y,z$
   
   $(m_{1} | 0,0,1/2)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

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<td>6</td>
<td>c</td>
<td>(1) x,y,z [u,v,w] (2) y,x,y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w] (4) y,x,z+1/2 [v,u,w] (5) x,y,z+1/2 [u-v,v,w] (6) x,x,y,z+1/2 [u,u+v,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>1/3,2/3,z [0,0,w] 2/3,1/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,z [0,0,w] 0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p31m'  
  \[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  
  Origin at 0,0,z

- Along [1,0,0] p1g'1  
  \[ \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]  
  Origin at x,0,0

- Along [2,1,0] p1  
  \[ \mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = \mathbf{b}/2 \]  
  Origin at x,x/2,0
Origin on 3m

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/3; \quad x \leq 2y; \quad y \leq \min(1-x,2x) \]

Vertices

\begin{align*}
0,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 \\
0,0,1/3 & \quad 2/3,1/3,1/3 & \quad 1/3,2/3,1/3
\end{align*}
Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0
(3) 3' 0,0,0
(3') 0,0,0
(3') 0,0,0
(2) 3' 0,0,0
(3) 3' 0,0,0
(3') 0,0,0
(4) m x,x,z
(mx 0,0,0)
(5) m x,2x,z
(mx 0,0,0)
(6) m 2x,x,z
(my 0,0,0)

For (2/3,1/3,1/3) + set

(1) t (2/3,1/3,1/3)
(1,2/3,1/3,1/3)
(2) 3' (0,0,1/3) 1/3,1/3,1/3
(3) 3' (0,0,1/3) 1/3,1/3,1/3
(3') 2/3,1/3,1/3
(4) g (1/6,-1/6,1/3) x+1/2,x,z
(my 2/3,1/3,1/3)
(5) g (1/6,1/3,1/3) x,2x-1/2,z
(mx 2/3,1/3,1/3)
(6) g (2/3,1/3,1/3) 2x,x,z
(my 2/3,1/3,1/3)

For (1/3,2/3,2/3) + set

(1) t (1/3,2/3,2/3)
(1,1/3,2/3,2/3)
(2) 3' (0,0,2/3) 0,1/3,1/3
(3) 3' (0,0,2/3) 0,1/3,1/3
(3') 1/3,2/3,2/3
(4) g (-1/6,1/6,2/3) x+1/2,x,z
(my 1/3,2/3,2/3)
(5) g (1/3,2/3,2/3) x,2x,z
(mx 1/3,2/3,2/3)
(6) g (1/3,1/6,2/3) 2x-1/2,x,z
(my 1/3,2/3,2/3)

Generators selected (1): t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

18       c        1
(0,0,0) +
(1) x,y,z [u,v,w]
(2) y,x-y,z [v,u-v,w]
(3) x+y,x,z [u+v,u,w]
(4) y,x,z [v,u,w]
(5) x+y,y,z [u-v,v,w]
(6) x,y-z [u,u+v,w]

9         b        .m
(0,0,0) +
(1) x,x,z [u,u,0]
(2) x,x,z [u,0,0]
(3) x,x,z [0,u,0]

3         a        3m
(0,0,0) +
(0,0,0)

Symmetry of Special Projections

Along [0,0,1] p31m
a^* = (2a + b)/3  b^* = (-a + 2b)/3
Origin at 0,0,z

Along [1,0,0] p11'
a^* = (-a - 2b + c)/3  b^* = (a + 2b)/2
Origin at x,0,0

Along [2,1,0] p1m1
a^* = b/2  b^* = c/3
Origin at x,x/2,0
Origin on 3m'  

Asymmetric unit  

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
<th>x</th>
<th>y</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2/3</td>
<td>1/3</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1/3</td>
<td>2/3</td>
<td>1/3</td>
</tr>
<tr>
<td>0</td>
<td>2/3</td>
<td>1/3</td>
<td>1/3</td>
<td>2/3</td>
</tr>
</tbody>
</table>

y \leq \min(1-x,2x)
Continued 160.2.1296

**Symmetry Operations**

For (0,0,0) + set

1. 1 (1,0,0)
2. $3^*$ (0,0,0) (0,0,0)$^*$
3. $3^*$ (0,0,0) (0,0,0)$^*$
4. $m_{xy}$ (0,0,0)
5. $m_{xy}$ (0,0,0)
6. $m_{xy}$ (0,0,0)

For (2/3,1/3,1/3) + set

1. $t$ (2/3,1/3,1/3) (2/3,1/3,1/3)$^*$
2. $3^*$ (0,0,1/3) (0,0,1/3)$^*$
3. $3^*$ (0,0,1/3) (0,0,1/3)$^*$
4. $g$ (1/6,-1/6,1/3) (1/6,-1/6,1/3)$^*$
5. $g$ (1/6,1/3,1/3) (1/6,1/3,1/3)$^*$
6. $g$ (2/3,1/3,1/3) (2/3,1/3,1/3)$^*$

For (1/3,2/3,2/3) + set

1. $t$ (1/3,2/3,2/3) (1/3,2/3,2/3)$^*$
2. $3^*$ (0,0,2/3) (0,0,2/3)$^*$
3. $3^*$ (0,0,2/3) (0,0,2/3)$^*$
4. $g$ (-1/6,1/6,2/3) (1/6,1/6,2/3)$^*$
5. $g$ (1/3,2/3,2/3) (1/3,2/3,2/3)$^*$
6. $g$ (1/3,1/6,2/3) (1/3,1/6,2/3)$^*$

For (0,0,0)' + set

1. $1'$ (0,0,0)$'$
2. $3^*$ (0,0,0)$'$ (0,0,0)$'$
3. $3^*$ (0,0,0)$'$ (0,0,0)$'$
4. $m_{xy}$ (0,0,0)$'$
5. $m_{xy}$ (0,0,0)$'$
6. $m_{xy}$ (0,0,0)$'$

For (2/3,1/3,1/3)' + set

1. $t'$ (2/3,1/3,1/3) (1/3,2/3,1/3)$'$
2. $3^*$ (0,0,1/3) (0,0,1/3)$'$
3. $3^*$ (0,0,1/3) (0,0,1/3)$'$
4. $g'$ (1/6,-1/6,1/3) (1/6,-1/6,1/3)$'$
5. $g'$ (1/6,1/3,1/3) (1/6,1/3,1/3)$'$
6. $g'$ (2/3,1/3,1/3) (2/3,1/3,1/3)$'$

For (1/3,2/3,2/3)' + set

1. $t'$ (1/3,2/3,2/3) (1/3,2/3,2/3)$'$
2. $3^*$ (0,0,2/3) (0,0,2/3)$'$
3. $3^*$ (0,0,2/3) (0,0,2/3)$'$
4. $g'$ (-1/6,1/6,2/3) (1/6,1/6,2/3)$'$
5. $g'$ (1/3,2/3,2/3) (1/3,2/3,2/3)$'$
6. $g'$ (1/3,1/6,2/3) (1/3,1/6,2/3)$'$

**Generators selected**

(1); $t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); $1'$. 

160.2.1296 - 3 - 2789
Continued

160.2.1296

R3m1'

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff Letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1,1/2,1/2) + (0,1/2,1/2) +</td>
<td>(2/3,1/3,1/3) + (1/3,2/3,2/3) +</td>
</tr>
<tr>
<td>(0,0,0)' + (1/3,2/3,2/3)' +</td>
<td>(2/3,1/3,1/3)' + (1/3,2/3,2/3)' +</td>
</tr>
</tbody>
</table>

18 c 11' (1) x,y,z [0,0,0] (2) y-x-y,z [0,0,0] (3) x+y,x,z [0,0,0]

(4) y-x,x,z [0,0,0] (5) x+y,y,z [0,0,0] (6) x,x-y,z [0,0,0]

9 b .m1' x,x,z [0,0,0] x,2x,z [0,0,0] 2x,x,z [0,0,0]

3 a 3m1' 0,0,z [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1] p31m1'

\(a^* = \frac{2a + b}{3}\)  \(b^* = \frac{-a + b}{3}\)

Origin at 0,0,z

Along [1,0,0] p11'

\(a^* = \frac{-a - 2b + c}{3}\)  \(b^* = \frac{a + 2b}{2}\)

Origin at x,0,0

Along [2,1,0] p1m11'

\(a^* = \frac{b}{2}\)  \(b^* = \frac{c}{3}\)

Origin at x,x/2,0
R3m' 3m' Trigonal
160.3.1297 R3m'
Origin on 3m'

Asymmetric unit

\begin{align*}
0 \leq x & \leq 2/3; & 0 \leq y & \leq 2/3; & 0 \leq z & \leq 1/3; & x & \leq 2y; & y \leq \min(1-x, 2x) \\
\text{Vertices} & & & & & & & \\
0,0,0 & 2/3,1/3,0 & 1/3,2/3,0 \\
0,0,1/3 & 2/3,1/3,1/3 & 1/3,2/3,1/3
\end{align*}
Symmetry Operations

For (0,0,0) + set

1. 1
   (1) (0,0,0)

2. 3' 0,0,z
   (2) 3* 0,0,z
   (3) 3* 0,0,z
   (1,0,0)
   (3,0,0)
   (3,0,0)

3. m' x,x,z
   (4) m' x,x,z
   (5) m' x,x,z
   (6) m' x,x,z
   (m_x,0,0)' (-1)
   (m_x,0,0)'
   (m_y,0,0)'

For (2/3,1/3,1/3) + set

1. t (2/3,1/3,1/3)
   (1) (2/3,1/3,1/3)
   (2) 3* (0,0,1/3) 1/3,1/3,z
   (3) 3* (0,0,1/3) 1/3,0,z
   (3,0,0,1/3)
   (3,0,0,1/3)
   (3,0,0,1/3)

2. g' (1/6,-1/6,1/3) x+1/2,x,z
   (4) g' (1/6,-1/6,1/3) x+1/2,x,z
   (5) g' (1/6,-1/6,1/3) x+1/2,x,z
   (6) g' (1/6,-1/6,1/3) x+1/2,x,z
   (m_x,1/3,1/3,1/3)'
   (m_x,1/3,1/3,1/3)'
   (m_x,1/3,1/3,1/3)'

For (1/3,2/3,2/3) + set

1. t (1/3,2/3,2/3)
   (1) (1/3,2/3,2/3)
   (2) 3* (0,0,2/3) 0,1/3,z
   (3) 3* (0,0,2/3) 0,1/3,z
   (3,0,2/3,0,1/3)
   (3,0,2/3,0,1/3)
   (3,0,2/3,0,1/3)

2. g' (-1/6,1/6,2/3) x+1/2,x,z
   (4) g' (-1/6,1/6,2/3) x+1/2,x,z
   (5) g' (-1/6,1/6,2/3) x+1/2,x,z
   (6) g' (-1/6,1/6,2/3) x+1/2,x,z
   (m_x,1/3,2/3,2/3)'
   (m_x,1/3,2/3,2/3)'
   (m_x,1/3,2/3,2/3)'

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>c</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x+y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x-y,z [u,u-v,w]</td>
</tr>
<tr>
<td>9</td>
<td>b</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,z [u,2u,w]</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,z [2u,u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m' Along [1,0,0] p1 Along [2,1,0] p1m'1

a*= (2a + b)/3  b*= (-a + b)/3  a* = (-a - 2b + c)/3  b* = (a + 2b)/2  a* = b/2  b* = c/3
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
Origin on 3m

Asymmetric unit

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0,0,0</th>
<th>2/3,1/3,0</th>
<th>1/3,2/3,0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0,0,1/3</td>
<td>2/3,1/3,1/3</td>
<td>1/3,2/3,1/3</td>
</tr>
</tbody>
</table>
Symmetry Operations

For (0,0,0) + set

(1) 1 (1) 0,0,0 (2) 3* 0,0,z (3) 3* 0,0,z
(3z) 0,0,0 (3z) 0,0,0

(4) m x,x,z (5) m x,2x,z (6) m 2x,x,z
(m_x,0,0) (m_x,0,0) (m_y,0,0)

For (2/3,1/3,1/3)' + set

(1) t' (2/3,1/3,1/3) (2) 3*'(0,0,1/3) 1/3,1/3,z (3) 3*'(0,0,1/3) 1/3,0,z (3z) 2/3,1/3,1/3)
(1/2,3,1/3,1/3)' (3z) 2/3,1/3,1/3)' (3z) 2/3,1/3,1/3)' (3z) 2/3,1/3,1/3)

(4) g' (1/6,-1/6,1/3) x+1/2,x,z (5) g'(1/6,1/3,1/3) x,2x-1/2,z (6) g'(2/3,1/3,1/3) 2x,x,z
(m_x,2/3,1/3,1/3)' (m_x,2/3,1/3,1/3)' (m_y,2/3,1/3,1/3)' (m_y,2/3,1/3,1/3)'

For (1/3,2/3,2/3) + set

(1) t (1/3,2/3,2/3) (2) 3* (0,0,2/3) 0,1/3,z (3) 3* (0,0,2/3) 1/3,1/3,z
(1/3,2/3,2/3) (3) 1/3,2/3,2/3) (3z) 1/3,2/3,2/3) (3z) 1/3,2/3,2/3)

(4) g (-1/6,1/6,2/3) x+1/2,x,z (5) g (1/3,2/3,2/3) x,2x,z (6) g (1/3,1/6,2/3) 2x-1/2,x,z
(m_x,1/3,2/3,2/3) (m_x,1/3,2/3,2/3) (m_x,1/3,2/3,2/3) (m_x,1/3,2/3,2/3)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3);(2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

(0,0,0) + (2/3,1,1/3)' + (1/3,2,2/3) +

18 c 1 (1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w]

(4) y,x,z [v,u,w] (5) x+y,y,z [u-v,v,w] (6) x-x,y,z [u,u+v,w]

9 b .m x,x,z [u,u,0] x,2x,z [u,0,0] 2x,x,z [0,u,0]

3 a 3m 0,0,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p31m1' Along [1,0,0] p11' Along [2,1,0] p2v 1m

a* = (2a+b)/3 b* = (a+b)/3 a* = (-a - 2b + c)/3 b* = (a + 2b)/2

Origin at 0,0,z Origin at 1,0,0 Origin at x,x/2,0
Origin on 3m'

Asymmetric unit

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0 ≤ x ≤ 2/3;</th>
<th>0 ≤ y ≤ 2/3;</th>
<th>0 ≤ z ≤ 1/3;</th>
<th>x ≤ 2y;</th>
<th>y ≤ min(1-x,2x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>2/3,1/3,0</td>
<td>1/3,2/3,0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,0,1/3</td>
<td>2/3,1/3,1/3</td>
<td>1/3,2/3,1/3</td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>
Symmetry Operations

For (0,0,0) + set

(1) 1 (2) 3' 0,0,z (3) 3' 0,0,z
     (1,0,0) (3,0,0,0) (3,0,0,0)

(4) m' x,x,z (5) m' x,2x,z (6) m' 2x,x,z
    (m_x',0,0,0') (m_x,0,0,0') (m_y,0,0,0')

For (2/3,1/3,1/3)' + set

(1) t' (2/3,1/3,1/3) (2) 3' ' (0,0,1/3) 1/3,1/3,z (3) 3' ' (0,0,1/3) 1/3,0,z
     (1,2/3,1/3,1/3)' (3,0,1/3,0,1/3)' (3,0,1/3,0,1/3)'

(4) g (1/6,-1/6,1/3) x+1/2,x,z (5) g (1/6,1/3,1/3) x,2x-1/2,z (6) g (2/3,1/3,1/3) 2x,x,z
    (m_x,2/3,1/3,1/3) (m_x,2/3,1/3,1/3) (m_y,2/3,1/3,1/3)

For (1/3,2,3/2,3) + set

(1) t (1/3,2,3/2,3) (2) 3' (0,0,2/3) 0,1/3,z (3) 3' (0,0,2/3) 1/3,1/3,z
     (1,1/3,2,3/2,3) (3,1/3,2,3,2/3) (3,1/3,2,3,2/3)

(4) g' (-1/6,1/6,2/3) x+1/2,x,z (5) g' (1/3,2,3/2,3) x,2x,z (6) g' (1/3,1/6,2/3) 2x-1/2,x,z
    (m_x,1/3,2,3,2/3) (m_x,1/3,2,3,2/3) (m_y,1/3,2,3,2/3)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3);(2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>c</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2/3,1,3/1/3)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1/3,2,3/2,3) +</td>
</tr>
<tr>
<td>9</td>
<td>b</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>.m'</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>3m'</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m'  
\( a^* = (2a + b)/3 \) \( b^* = (-a + b)/3 \)
Origin at 0,0,z

Along [1,0,0] \( p_{3\alpha} \)
\( a^* = (-a - 2b + c)/3 \) \( b^* = (a + 2b)/2 \)
Origin at x,0,0

Along [2,1,0] \( p_{2\nu} \)
\( a^* = b/2 \) \( b^* = c/3 \)
Origin at x,x/2,0
Origin on 3c

Asymmetric unit: $0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$

Vertices:
- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/6$
- $1/2,0,1/6$
- $2/3,1/3,1/6$
- $1/3,2/3,1/6$
- $0,1/2,1/6$
Symmetry Operations

For $(0,0,0)$ + set

1. $1 (0,0,0)$
2. $3^* 0,0,z (3,0,0,0)$
3. $3^* 0,0,z (3,z,0,0)$
4. $c (0,0,1/2) x,x,z (m_x|0,0,1/2)$
5. $c (0,0,1/2) x,2x,z (m_x|0,0,1/2)$
6. $c (0,0,1/2) 2x,x,z (m_y|0,0,1/2)$

For $(2/3,1/3,1/3)$ + set

1. $t (2/3,1/3,1/3) (1/2,3,1/3,1/3)$
2. $3^* (0,0,1/3) 1/3,1/3,z (3,z,2/3,1/3,1/3)$
3. $3^* (0,0,1/3) 1/3,0,z (3,z,2/3,1/3,1/3)$
4. $g (1/6,1/6,1/6) x+1/2,x,z (m_y|2/3,1/3,5/6)$
5. $g (1/6,1/3,1/6) x,2x-1/2,z (m_y|2/3,1/3,5/6)$
6. $g (2/3,1/3,1/6) 2x,x,z (m_y|2/3,1/3,5/6)$

For $(1/3,2/3,1/3)$ + set

1. $t (1/3,2/3,1/3) (1/1,3,2/3,2/3)$
2. $3^* (0,0,2/3) 0,1/3,z (3,z,1/3,2/3,2/3)$
3. $3^* (0,0,2/3) 1/3,1/3,z (3,z,1/3,2/3,2/3)$
4. $g (-1/6,1/6,1/6) x+1/2,x,z (m_y|1/3,2/3,3,1/6)$
5. $g (1/3,2/3,1/6) x,2x,z (m_y|1/3,2/3,3,1/6)$
6. $g (1/3,1/6,1/6) 2x-1/2,x,z (m_y|1/3,2/3,3,1/6)$

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>b 1</td>
<td>(1) (x, y, z [u, v, w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) ( y, x-y, z [v, u-v, w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) (x+y, x, z [u+v, u, w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) ( y, x, z+1/2 [v, u, w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) (x+y, y, z+1/2 [u-v, v, w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) (x, x+y, z+1/2 [u, u+v, w])</td>
</tr>
<tr>
<td>3</td>
<td>a 3</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \(p31m\)
\(a^* = (2a + b)/3\)
Original at \(0,0,z\)

Along \([1,0,0]\) \(p_{2\bar{1}}\)
\(a^* = (2a + 4b + c)/6\)
Origin at \(x,0,0\)

Along \([2,1,0]\) \(p1g1\)
\(a^* = b/2\)
Origin at \(x,x/2,0\)
Origin on 3c1'

Asymmetric unit

<table>
<thead>
<tr>
<th></th>
<th>0 ≤ x ≤ 2/3;</th>
<th>0 ≤ y ≤ 2/3;</th>
<th>0 ≤ z ≤ 1/6;</th>
<th>x ≤ (1+y)/2;</th>
<th>y ≤ min(1-x,(1+x)/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices</td>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
<td>1/3,2/3,0</td>
<td>0,1/2,0</td>
</tr>
<tr>
<td></td>
<td>0,0,1/6</td>
<td>1/2,0,1/6</td>
<td>2/3,1/3,1/6</td>
<td>1/3,2/3,1/6</td>
<td>0,1/2,1/6</td>
</tr>
</tbody>
</table>
Symmetry Operations

For (0,0,0) + set

(1) \text{t}(0,0,0)  \\
(2) 3^* 0,0,z  \\
(3) 3^* 0,0,z  \\
(4) c(0,0,1/2) x,x,z  \\
(5) c(0,0,1/2) x,2x,z  \\
(6) c(0,0,1/2) 2x,x,z

For (2/3,1/3,1/3) + set

(1) \text{t}(2/3,1/3,1/3)  \\
(2) 3^* (0,0,1/3) 1/3,1/3,z  \\
(3) 3^* (0,0,1/3) 1/3,0,z  \\
(4) g(1/6,-1/6,5/6) x+1/2,x,z  \\
(5) g(1/6,1/3,5/6) x,2x-1/2,z  \\
(6) g(2/3,1/3,5/6) 2x,x,z

For (1/3,2,3/2) + set

(1) \text{t}(1/3,2,3/2)  \\
(2) 3^* (0,0,2/3) 0,1/3,z  \\
(3) 3^* (0,0,2/3) 1/3,1/3,z  \\
(4) g(-1/6,1/6,1/6) x+1/2,x,z  \\
(5) g(1/3,2,3/2,1/6) x,2x,z  \\
(6) g(1/3,1/6,1/6) 2x-1/2,x,z

For (0,0,0)' + set

(1) \text{t}(0,0,0)'  \\
(2) 3^* 0,0,z  \\
(3) 3^* 0,0,z  \\
(4) c'(0,0,1/2) x,x,z  \\
(5) c'(0,0,1/2) x,2x,z  \\
(6) c'(0,0,1/2) 2x,x,z

For (2/3,1/3,1/3)' + set

(1) \text{t}'(2/3,1/3,1/3)  \\
(2) 3^*' (0,0,1/3) 1/3,1/3,z  \\
(3) 3^*' (0,0,1/3) 1/3,0,z  \\
(4) g'(1/6,-1/6,5/6) x+1/2,x,z  \\
(5) g'(1/6,1/3,5/6) x,2x-1/2,z  \\
(6) g'(2/3,1/3,5/6) 2x,x,z

For (1/3,2,3/2)'+ set

(1) \text{t}'(1/3,2,3/2)  \\
(2) 3^*' (0,0,2/3) 0,1/3,z  \\
(3) 3^*' (0,0,2/3) 1/3,1/3,z  \\
(4) g'(-1/6,1/6,1/6) x+1/2,x,z  \\
(5) g'(1/3,2,3/2,1/6) x,2x,z  \\
(6) g'(1/3,1/6,1/6) 2x-1/2,x,z

Generators selected (1); 
(1,0,0); 
(0,0,1); 
(2/3,1/3,1/3); (2); 
(4); 1'.
Continued

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +
(0,0,0)' + (2/3,1/3,1/3)' + (1/3,2/3,2/3)' +

18 b 11' (1) x,y,z [0,0,0] (2) y,x-y,z [0,0,0] (3) x+y,x ,z [0,0,0]
(4) y,x,z+1/2 [0,0,0] (5) x+y,y,z+1/2 [0,0,0] (6) x,x-y,z+1/2 [0,0,0]

3 a 3.1' 0,0,z [0,0,0] 0,0,z+1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p31m1' a* = (2a + b)/3 b* = (-a + b)/3
Origin at 0,0,z
Along [1,0,0] p11' a* = (2a + 4b + c)/6 b* = (a + 2b)/2
Origin at x,0,0
Along [2,1,0] p1g11' a* = b/2 b* = c/3
Origin at x,x/2,0
R3c'  3m'  Trigonal

161.3.1302  161.3.1302 R3c'
Origin on 3c'

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{6}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,\frac{1+x}{2}) \]

Vertices

\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/6 & \quad 1/2,0,1/6 & \quad 2/3,1/3,1/6 & \quad 1/3,2/3,1/6 & \quad 0,1/2,1/6
\end{align*}
Symmetry Operations

For (0,0,0) + set

(1) \(1\) \((0,0,0)\)
(2) \(3^+ 0,0,z\)
(3) \(3^- 0,0,z\)
(4) \(c' (0,0,1/2) x,x,z\)
\((m_x|0,0,1/2)'\)

For (2/3,1/3,1/3) + set

(1) \(t (2/3,1/3,1/3)\)
(2) \(3^+ (0,0,1/3) 1/3,1/3,z\)
(3) \(3^- (0,0,1/3) 1/3,0,z\)
(4) \(g' (1/6,-1/6,5/6) x+1/2,x,z\)
\((m_x|2/3,1/3,5/6)'\)

For (1/3,2/3,2/3) + set

(1) \(t (1/3,2/3,2/3)\)
(2) \(3^+ (0,0,2/3) 0,1/3,z\)
(3) \(3^- (0,0,2/3) 1/3,1/3,z\)
(4) \(g' (-1/6,1/6,1/6) x+1/2,x,z\)
\((m_x|1/3,2/3,1/6)'\)

Generators selected

(1): \((1,0,0); (0,1,0); (t(0,0,1); t(2/3,1/3,1/3);(2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 b 1</td>
<td>0,0,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\tilde{y},x-y,z) ([v,u-v,w])</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\tilde{x}+y,x,z) ([u+v,u,w])</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(\tilde{y},x,z+1/2) ([v,u,w])</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(x,y,z+1/2) ([u,v+w])</td>
<td></td>
</tr>
<tr>
<td>3 a 3.</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \(p31m'\)
\(a^* = (2a+b)/3\) \(b^* = (-a+b)/3\)
Origin at 0,0,z

Along [1,0,0] \(p1\)
\(a^* = (2a+4b+c)/6\) \(b^* = (a+2b)/2\)
Origin at x,0,0

Along [2,1,0] \(p1g'1\)
\(a^* = b/2\) \(b^* = c/3\)
Origin at x,x/2,0
**Origin** on center (31m)

**Asymmetric unit**

| 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ (1+y)/2; y ≤ min(1-x,x) |
|---------------------------------|---|---|---|---|
| Vertices | 0,0,0 | 1/2,0,0 | 2/3,1/3,0 | 1/2,1/2,0 |
|           | 0,0,1/2 | 1/2,0,1/2 | 2/3,1/3,1/2 | 1/2,1/2,1/2 |

**Symmetry Operations**

(1) 1
(2) 3⁺ 0,0,z
(3) 3⁻ 0,0,z
(4) 2 x,x,0
(5) 2 x,2x,0
(6) 2 2x,x,0
(7) 1⁻ 0,0,0
(8) 3⁺ 0,0,z; 0,0,0
(9) 3⁻ 0,0,z; 0,0,0
(10) m x,x,z
(11) m x,0,z
(12) m 0,y,z
162.1.1303

**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity,</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>(x,y,z {u,v,w})</td>
</tr>
<tr>
<td>(2)</td>
<td>(\bar{y},x-y,z {\bar{v},u-v,w})</td>
</tr>
<tr>
<td>(3)</td>
<td>(\bar{x}+y,\bar{x},z {\bar{u}+\bar{v},\bar{u},w})</td>
</tr>
<tr>
<td>(4)</td>
<td>(\bar{y},x,\bar{z} {\bar{v},u,w})</td>
</tr>
<tr>
<td>(5)</td>
<td>(\bar{x}+y,y,x {\bar{v},\bar{u},w})</td>
</tr>
<tr>
<td>(6)</td>
<td>(\bar{y},x,\bar{z} {\bar{v},\bar{u},w})</td>
</tr>
<tr>
<td>(7)</td>
<td>(\bar{x},\bar{y},\bar{z} {\bar{u},v,w})</td>
</tr>
<tr>
<td>(8)</td>
<td>(\bar{y},x,\bar{z} {\bar{v},\bar{u},w})</td>
</tr>
<tr>
<td>(9)</td>
<td>(\bar{x},\bar{y},\bar{z} {\bar{u}+\bar{v},\bar{u},w})</td>
</tr>
<tr>
<td>(10)</td>
<td>(\bar{y},x,\bar{z} {\bar{v},\bar{u},w})</td>
</tr>
<tr>
<td>(11)</td>
<td>(\bar{x},\bar{y},\bar{z} {\bar{u}+\bar{v},\bar{u},w})</td>
</tr>
<tr>
<td>(12)</td>
<td>(\bar{x},\bar{y},\bar{z} {\bar{u},v,w})</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**  
  \(p6\hat{m1}m\)  
  \(a^* = a\)  
  \(b^* = b\)  
- **Along [1,0,0]**  
  \(p2\hat{m}1\hat{m}\)  
  \(a^* = (a+2b)/2\)  
  \(b^* = c\)  
- **Along [2,1,0]**  
  \(p2111\)  
  \(a^* = c\)  
  \(b^* = b/2\)  

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x/2,0
Origin on center (31m1')

Asymmetric unit

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1/2</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1/2</td>
</tr>
<tr>
<td>1/2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1/2</td>
<td>1/2</td>
<td>0</td>
</tr>
<tr>
<td>1/2</td>
<td>1/2</td>
<td>1/2</td>
</tr>
</tbody>
</table>

Symmetry Operations

For $1 +$ set

1. $1$
   
2. $3^+$ 0,0,0
   
3. $3^-$ 0,0,0
   
4. $2x$, ,0
   
5. $2x$,2x,0
   
6. $2x$, ,0
   
7. $3^-$ 0,0,0
   
8. $3^-$ 0,0,0
   
9. $3^-$ 0,0,0
   
10. $m$,x,z

11. $m$,x,0

12. $m$,y,z
For \(1' + \) set

\[
\begin{align*}
(1) & \quad 1' \quad (11') \quad (0,0,0)' \\
(2) & \quad 3' \quad 0,0,z \quad (3_2') \quad (0,0,0)' \\
(3) & \quad 3' \quad 0,0,z \quad (3_2') \quad (0,0,0)' \\
(4) & \quad 2' \quad x,x,0 \quad (2_2') \quad (0,0,0)' \\
(5) & \quad 2' \quad x,2x,0 \quad (2_2') \quad (0,0,0)' \\
(6) & \quad 2' \quad 2x,x,0 \quad (2_2') \quad (0,0,0)' \\
(7) & \quad 1' \quad (11') \quad (0,0,0)' \\
(8) & \quad 3' \quad 0,0,z; 0,0,0 \quad (3_2') \quad (0,0,0)' \\
(9) & \quad 3' \quad 0,0,z; 0,0,0 \quad (3_2') \quad (0,0,0)' \\
(10) & \quad m' \quad x,x,z \quad (m_2') \quad (0,0,0)' \\
(11) & \quad m' \quad x,0,z \quad (m_2') \quad (0,0,0)' \\
(12) & \quad m' \quad 0,y,z \quad (m_2') \quad (0,0,0)' \\
\end{align*}
\]

Generators selected

\(1\); \(t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); \(1'\).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 (l) (11')</td>
<td>(1) ((x,y,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(2) ((y,x-y,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(3) ((x+y,0,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(4) ((y,x,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(5) ((x+y,y,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(6) ((x,y,x) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(7) ((x+y,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(8) ((y,x+y,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(9) ((x,y,x) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(10) ((y,x,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(11) ((x+y,y,z) [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(12) ((x,x+y,z) [0,0,0])</td>
</tr>
<tr>
<td>6 (k) (.m1')</td>
<td>(x,0,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(0,x,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(0,x,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(x,0,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(x,x,z [0,0,0])</td>
</tr>
<tr>
<td>6 (j) (.21')</td>
<td>(x,x,1/2 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(x,1/2,1/2 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(x,2x,1/2 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(2x,x,1/2 [0,0,0])</td>
</tr>
<tr>
<td>6 (i) (.21')</td>
<td>(x,x,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(x,2x,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(x,2x,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(2x,x,0 [0,0,0])</td>
</tr>
<tr>
<td>4 (h) (.3,1')</td>
<td>(1/3,2/3,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(1/3,2/3,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(2/3,1/3,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(2/3,1/3,z [0,0,0])</td>
</tr>
<tr>
<td>3 (g) (.2/m1')</td>
<td>(1/2,0,1/2 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(0,1/2,1/2 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,1/2 [0,0,0])</td>
</tr>
<tr>
<td>3 (f) (.2/m1')</td>
<td>(1/2,0,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(0,1/2,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,0 [0,0,0])</td>
</tr>
<tr>
<td>2 (e) (3.m1')</td>
<td>(0,0,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(0,0,z [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(0,0,z [0,0,0])</td>
</tr>
<tr>
<td>2 (d) (3.21')</td>
<td>(1/3,2/3,1/2 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(2/3,1/3,1/2 [0,0,0])</td>
</tr>
<tr>
<td>2 (c) (3.21')</td>
<td>(1/3,2/3,0 [0,0,0])</td>
</tr>
<tr>
<td></td>
<td>(2/3,1/3,0 [0,0,0])</td>
</tr>
<tr>
<td>1 (b) (3.m1')</td>
<td>(0,0,1/2 [0,0,0])</td>
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<td>(0,0,1/2 [0,0,0])</td>
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Continued

Synergy of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Symmetry</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p6mm1'</td>
<td>a* = a, b* = b</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2mm1'</td>
<td>a* = c, b* = (a + 2b)/2</td>
</tr>
<tr>
<td>Along [2,1,0]</td>
<td>p2111'</td>
<td>a* = c, b* = b/2</td>
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</table>

Origin at 0,0,z
Origin at x,0,0
Origin at x,x/2,0
Origin on center (3'1m)

Asymmetric unit

<table>
<thead>
<tr>
<th></th>
<th>0 ≤ x ≤ 2/3;</th>
<th>0 ≤ y ≤ 1/2;</th>
<th>0 ≤ z ≤ 1/2;</th>
<th>x ≤ (1+y)/2;</th>
<th>y ≤ min(1-x,x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
<td>1/2,1/2,0</td>
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<td></td>
</tr>
<tr>
<td>0,0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1/3,1/2</td>
<td>1/2,1/2,1/2</td>
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</tr>
</tbody>
</table>

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 3' 0,0,z
(3' | 0,0,0)

(3) 3' 0,0,z
(3' | 0,0,0)

(4) 2' x,x,0
(2 | 0,0,0)
(2 | 0,0,0)

(5) 2' x,2x,0
(2 | 0,0,0)
(2 | 0,0,0)

(6) 2' 2x,x,0
(2 | 0,0,0)
(2 | 0,0,0)

(7) 3' 0,0,z
(3' | 0,0,0)

(8) 3' 0,0,z
(3' | 0,0,0)

(9) 3' 0,0,z
(3' | 0,0,0)

(10) m x,x,z
(m | 0,0,0)

(11) m x,0,z
(m | 0,0,0)

(12) m 0,y,z
(m | 0,0,0)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>l</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v-u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
<td>(5) x+y,y,z [u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
<td>(8) y,x+y,z [u,v+w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y,x,z [v,0,w]</td>
<td>(11) x-y,y,z [u+v,0]</td>
</tr>
<tr>
<td>6</td>
<td>k</td>
<td>x',0,z [u,2u,0]</td>
<td>0,x,z [2u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,x',z [2u,0,0]</td>
<td>x',0,z [u,2u,0]</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>x',1/2 [u,u,0]</td>
<td>x,2x,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x',x,1/2 [u,u,0]</td>
<td>x',2x,1/2 [u,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>x',0 [u,u,0]</td>
<td>x,2x,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x',x,0 [u,u,0]</td>
<td>x',2x,0 [u,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>1/3,2/3,z [0,0,0]</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>f</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>1/3,2/3,0 [0,0,0]</td>
<td>2/3,1/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p6mm
- **Along [1,0,0]**: p2mm
- **Along [2,1,0]**: p2111'

**Symmetry Operators**

- **a** = **a**  \( \mathbf{b}^* = \mathbf{b} \)
- **a** = **c**  \( \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)
- **a** = **c**  \( \mathbf{b}^* = \mathbf{b}/2 \)

- Origin at 0,0,z
- Origin at x,0,0
- Origin at x,x/2,0
**Origin** on center (3'1m')

**Asymmetric unit**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ (1+y)/2; y ≤ min(1-x,x)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Vertices**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
</tr>
<tr>
<td>0,0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1/3,1/2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,1/2,1/2</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. 1
2. 3' 0,0,z
3. 3' 0,0,z
4. 2 x,x,0
5. 2 x,2x,0
6. 2 2x,x,0
7. 1 0,0,0'
8. 3' ' 0,0,z; 0,0,0
9. 3' ' 0,0,z; 0,0,0
10. m' x,x,z
11. m' x,0,z
12. m' 0,y,z

162.4.1306 - 1 - 2817
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7)\).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>l</td>
</tr>
<tr>
<td>(4) y,x,z [v,u,w]</td>
<td>(5) x+y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td>(7) x,y,z [u,v,w]</td>
<td>(8) y,x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td>(10) y,x,z [v,u,w]</td>
<td>(11) x-y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td>6</td>
<td>k</td>
</tr>
<tr>
<td>0,x,z [0,u,w]</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
</tr>
<tr>
<td>x,x,1/2 [u,u,0]</td>
<td>x,2x,1/2 [u,2u,0]</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
</tr>
<tr>
<td>x,x,0 [u,u,0]</td>
<td>x,2x,0 [u,2u,0]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
</tr>
<tr>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
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<td>3</td>
<td>f</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- **Along [0,0,1]** \(p6m'm'\)  
  - \(a^* = a\) \(b^* = b\)  
  - Origin at 0,0,z
- **Along [1,0,0]** \(p2m'm'\)  
  - \(a^* = c\) \(b^* = (a + 2b)/2\)  
  - Origin at x,0,0
- **Along [2,1,0]** \(p211\)  
  - \(a^* = c\) \(b^* = b/2\)  
  - Origin at x,x/2,0
Origin on center (\(\overline{3}1m'\))

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1|0,0,0) \\
(1) & \quad (0,x,x,0) \\
(4) & \quad (2,0,0,0)' \\
(5) & \quad (2x,0,0,0)' \\
(7) & \quad (1,0,0,0) \\
(8) & \quad (3,0,0,0) \\
(10) & \quad (m,0,0,0)' \\
(11) & \quad (m,0,0,0)' \\
(12) & \quad (m,0,0,0)'
\end{align*}
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
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<th>Multiplicity</th>
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<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>l</td>
<td>1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-z [v,u-w] (3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) y,x,z [v,u-w] (5) x+y,y,z [v-u-w] (6) x-x,y,z [u,u+v,w]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(7) x+y,x,z [u+v,u-w] (10) y,x,z [v,u-w]</td>
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<tr>
<td></td>
<td>k</td>
<td>-m'</td>
<td>6</td>
</tr>
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<td></td>
<td></td>
<td>0,x,z [0,u,w]</td>
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<td>j</td>
<td>-2'</td>
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<td>x,2x,0 [0,u,w]</td>
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<td>x,0,2x [0,u,w]</td>
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<td>x,2x,0 [0,u,w]</td>
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<td>h</td>
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<td>4</td>
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<td>1/3,2/3,z [0,0,w]</td>
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<td>1/3,2/3,z [0,0,w]</td>
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<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
<td>.2'/m'</td>
<td>3</td>
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<td>1,2/0,1/2 [0,u,w]</td>
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<td>0,1,2/0 [0,u,w]</td>
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<td>0,1,2/0 [0,u,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<tr>
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<td>d</td>
<td>3.2'</td>
<td>2</td>
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<td>1/3,2/3,1/2 [0,0,w]</td>
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<td>2/3,1/3,1/2 [0,0,w]</td>
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<tr>
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<td></td>
<td>1/3,2/3,0 [0,0,w]</td>
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<td>2/3,1/3,0 [0,0,w]</td>
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<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
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<td>3.m'</td>
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<tr>
<td></td>
<td></td>
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<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1], p6mm'
Along [1,0,0], p2mm'
Along [2,1,0], p2'11
a* = a b* = b
a* = c b* = (a + 2b)/2
Origin at 0,0,z
Origin at x,0,0
Origin at x,x/2,0
**Origin** on center (31m)

**Asymmetric unit**

\[
0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,x)
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

**Symmetry Operations**

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad \text{1} & \quad (2) & \quad 3^* & \quad 0,0,z \\
& \quad (1|0,0,0) & \quad & \quad (3_z|0,0,0) & \quad (3_{z}^{-1}|0,0,0) \\
(4) & \quad 2 & \quad x,x,0 & \quad (2_z|0,0,0) & \quad (2_{z}^{-1}|0,0,0) \\
& \quad (2|0,0,0) & \quad & \quad (2_{z}|0,0,0) & \quad (2_{z}^{-1}|0,0,0) \\
(7) & \quad \overline{1} & \quad (1|0,0,0) & \quad (8) & \quad 3^* & \quad 0,0,z; 0,0,0 \\
& \quad (1|0,0,0) & \quad & \quad (3_z|0,0,0) & \quad (3_{z}^{-1}|0,0,0) \\
(10) & \quad m & \quad x,x,z & \quad (m_{3}|0,0,0) & \quad (11) & \quad m & \quad x,0,z & \quad (m_{2}|0,0,0) \\
& \quad (m_{3}|0,0,0) & \quad & \quad (m_{2}|0,0,0) & \quad & \quad (m_{1}|0,0,0) \quad (12) & \quad m & \quad 0,y,z \\
& \quad (m_{3}|0,0,0) & \quad & \quad (m_{2}|0,0,0) & \quad & \quad (m_{1}|0,0,0)
\end{align*}
\]
Continued

For $(0,0,1)^\prime$ +set

$\begin{align*}
(1) & t'(0,0,1) \\
(2) & (0,0,1)^\prime \quad (3) & 3 \cdot (0,0,1) \quad 0,0,z \\
(4) & 2' \, x,x,1/2 \\
(5) & 2' \, x,2x,1/2 \\
(6) & 2' \, 2x,x,1/2 \\
(4) & \bar{T} \, 0,0,1/2 \\
(5) & 3^{+} \cdot 0,0,z; \, 0,0,1/2 \\
(6) & 3^{+} \cdot 0,0,z; \, 0,0,1/2 \\
(4) & c' (0,0,1) \quad x,x,z \\
(5) & c' (0,0,1) \quad x,0,z \\
(6) & c' (0,0,1) \quad 0,y,z \\
\end{align*}$

Generators selected

$(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7)$.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>l</td>
<td>$(0,0,0) + (0,0,1)^\prime$</td>
</tr>
</tbody>
</table>

$\begin{align*}
(1) & x,y,z \, [v,u,w] \\
(2) & \bar{y},x-y,z \, [\bar{v},u-v,w] \\
(3) & x+y,\bar{x},z \, [u+v,\bar{u},w] \\
(4) & \bar{y},x,z \, [\bar{v},u,w] \\
(5) & x+y,y,z \, [u+v,v,w] \\
(6) & x,x-y,z \, [u-v,\bar{u},w] \\
(7) & x,y,z \, [v,u,w] \\
(8) & y,x+y,z \, [v,u-v,w] \\
(9) & x-y,x,z \, [u+v,\bar{u},w] \\
(10) & y,x,z \, [v,u,w] \\
(11) & x-y,\bar{y},z \, [u+v,v,w] \\
(12) & x,x,1/2 \, [u,v,0] \\
(13) & x,2x,1/2 \, [u,v,0] \\
(14) & x,2x,0 \, [u,v,0] \\
(15) & x,2x,1/2 \, [u,v,0] \\
(16) & x,2x,0 \, [u,v,0] \\
\end{align*}$

$\begin{align*}
12 & k \quad .m \quad x,0,z \, [2u,0] \\
(17) & 0,\bar{x},z \, [2u,\bar{u},0] \\
(18) & \bar{x},z \, [u,0] \\
12 & j \quad .2' \quad x,x,1/2 \, [u,u,w] \\
(19) & \bar{x},2x,1/2 \, [\bar{u},0,w] \\
(20) & 2x,2x,1/2 \, [u,w] \\
12 & i \quad .2 \quad x,x,0 \, [u,\bar{u},0] \\
(21) & x,2x,0 \, [u,\bar{u},0] \\
(22) & 2x,2x,0 \, [u,\bar{u},0] \\
(23) & 2x,2x,1/2 \, [u,\bar{u},0] \\
8 & h \quad 3.. \quad 1/3,2/3,z \, [0,0,w] \\
(24) & 1/3,2/3,z \, [0,0,w] \\
(25) & 2/3,1/3,z \, [0,0,w] \\
(26) & 2/3,1/3,z \, [0,0,w] \\
6 & g \quad .2'm \quad 1/2,0,1/2 \, [0,0,0] \\
(27) & 0,1/2,1/2 \, [0,0,0] \\
(28) & 1/2,1/2,1/2 \, [0,0,0] \\
6 & f \quad .2'm \quad 1/2,0,0 \, [2u,0] \\
(29) & 0,1/2,0 \, [2u,\bar{u},0] \\
(30) & 1/2,1/2,0 \, [u,\bar{u},0] \\
2 & e \quad 3.m \quad 0,0,z \, [0,0,0] \\
(31) & 0,0,\bar{z} \, [0,0,0] \\
4 & d \quad 3.2 \quad 1/3,2/3,1/2 \, [0,0,0] \\
(32) & 2/3,1/3,1/2 \, [0,0,0] \\
4 & c \quad 3.2 \quad 1/3,2/3,0 \, [0,0,0] \\
(33) & 2/3,1/3,0 \, [0,0,0] \\
2 & b \quad 3.m \quad 0,0,1/2 \, [0,0,0] \\
\end{align*}$
Symmetry of Special Projections

Along [0,0,1]  p6mm1'
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
Origin at 0,0,z

Along [1,0,0]  p2\(a^*\) 2mm
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)
Origin at x,0,1/2

Along [2,1,0]  p2111'
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)
Origin at x,x/2,0
Origin on center (31m')

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq \frac{2}{3}; & 0 \leq y & \leq \frac{1}{2}; & 0 \leq z & \leq \frac{1}{2}; & x & \leq \frac{(1+y)}{2}; & y & \leq \min(1-x,x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/2,1/2,0 \\
0,0,1/2 & & 1/2,0,1/2 & & 2/3,1/3,1/2 & & 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \ 1 & \ (2) & \ 3^z & \ 0,0,z & \ (3) & \ 3^{-1} & \ 0,0,z \\
(1|0,0,0) & & (3|0,0,0) & & (3|0,0,0)
\end{align*}
\]

\[
\begin{align*}
(4) & \ 2' & \ x,x,0 & \ (5) & \ 2' & \ x,2x,0 & \ (6) & \ 2' & \ 2x,x,0 \\
(2_3|0,0,0)' & & (2_3|0,0,0)' & & (2|0,0,0)'
\end{align*}
\]

\[
\begin{align*}
(7) & \ 1 & \ (8) & \ 3^z & \ 0,0,z & \ 0,0,0 & \ (9) & \ 3^{-1} & \ 0,0,z & \ 0,0,0 \\
(1|0,0,0) & & (3|0,0,0) & & (3|0,0,0)
\end{align*}
\]

\[
\begin{align*}
(10) & \ m' & \ x,x,z & \ (11) & \ m' & \ x,0,z & \ (12) & \ m' & \ 0,y,z \\
(m_3|0,0,0)' & & (m_3|0,0,0)' & & (m_1|0,0,0)'
\end{align*}
\]

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For \((0,0,1)\) + set

\[
\begin{align*}
(1) & \ t'(0,0,1) \\
(1) & \ t'(0,0,1) \\
(2) & \ 3' + (0,0,1) \ 0,0,z \\
(3) & \ 3' + (0,0,1) \ 0,0,z \\
(4) & \ x,\bar{x},1/2 \\
(2) & \ 2x,2x,1/2 \\
(5) & \ 2x,0,1/2 \\
(6) & \ 2x,2x,1/2 \\
(4) & \ \bar{T} \ 0,0,1/2 \\
(2) & \ 3^{-1} \ 0,0,1/2 \\
(3) & \ 3^{-1} \ 0,0,1/2 \\
4 & \ c(0,0,1) \ x,x,z \\
(3) & \ c(0,0,1) \ x,0,z \\
(2) & \ c(0,0,1) \ 0,y,z
\end{align*}
\]

**Generators selected** \( (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7). \)

**Positions**

- **Multiplicity, Wyckoff letter, Site Symmetry.**
  - **Coordinates**
  - **(0,0,0) + (0,0,1) +**

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>((0,0,0) + ) ((0,0,1) +)</td>
</tr>
<tr>
<td>24</td>
<td>l 1</td>
<td>(1) (x,y,z) [u,v,w] (2) (\bar{y},x-y,z) (\bar{u},v,w) (3) (x+y,\bar{x},z) (u+v,\bar{u},w)</td>
</tr>
<tr>
<td></td>
<td>(4) (\bar{y},x,z) [v,u,w] (5) (x+y,y,z) [u-v,v,w] (6) (x,x-y,z) [v-u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) (x,y,z) [u,v,w] (8) (y,x+y,z) [v,u-v,v,w] (9) (x+y,x,\bar{z}) [u+v,u,\bar{w}]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(10) (x,y,z) [v,u,w] (11) (x-y,y,z) [u-v,v,\bar{w}] (12) (\bar{x},x+y,z) [\bar{u},u+v,\bar{w}]</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>k ..m'</td>
<td>(x,0,z) [u,0,w] (0,0,\bar{z}) [u,0,w] (\bar{x},\bar{x},z) [\bar{u},\bar{u},w]</td>
</tr>
<tr>
<td></td>
<td>(0,0,\bar{z}) [u,0,w] (\bar{x},0,\bar{z}) [\bar{u},\bar{u},w] (x,\bar{x},z) [\bar{u},\bar{u},w]</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>j ..2</td>
<td>(x,\bar{x},1/2) [u,0,0] (x,2x,1/2) [u,2u,0] (2x,\bar{x},1/2) [2u,\bar{u},0]</td>
</tr>
<tr>
<td></td>
<td>(x,\bar{x},1/2) [u,0,0] (\bar{x},2x,1/2) [\bar{u},2\bar{u},0] (2x,\bar{x},1/2) [2u,0,0]</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>i ..2'</td>
<td>(x,\bar{x},0) [u,u,w] (x,2x,0) [u,0,w] (2x,\bar{x},0) [0,\bar{u},w]</td>
</tr>
<tr>
<td></td>
<td>(\bar{x},x,0) [u,u,w] (\bar{x},2x,0) [\bar{u},0,w] (2x,\bar{x},0) [0,\bar{u},w]</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>h 3..</td>
<td>1/3,2/3,\bar{z} [0,0,w] (2/3,2/3,\bar{z}) [0,0,w] (2/3,1/3,\bar{z}) [0,0,w] (2/3,1/3,\bar{z}) [0,0,w]</td>
</tr>
<tr>
<td>6</td>
<td>g ..2/m'</td>
<td>1/2,0,1/2 [0,0,0] (0,1/2,1/2) [0,0,0] (1/2,1/2,1/2) [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>f ..2'/m'</td>
<td>1/2,0,0 [u,0,w] (0,1/2,0) [u,0,w] (1/2,1/2,0) [\bar{u},\bar{w},w]</td>
</tr>
<tr>
<td>4</td>
<td>e 3.m'</td>
<td>0,0,\bar{z} [0,0,w] (0,0,\bar{z}) [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>d 3.2'</td>
<td>1/3,2/3,1/2 [0,0,w] (2/3,1/3,1/2) [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>c 3.2'</td>
<td>1/3,2/3,0 [0,0,w] (2/3,1/3,0) [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b ..3,m'</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] \( \text{p}6\text{mm}1' \)
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] \( \text{p}2\text{a}* \text{2m}' \text{m}' \)
\( a^* = c \quad b^* = (a + 2b)/2 \)
Origin at x,0,1/2

Along [2,1,0] \( \text{p}2\text{a}* \text{211} \)
\( a^* = c \quad b^* = b/2 \)
Origin at x,x/2,0
**Origin** at center (3) at $\bar{3}1c$

**Asymmetric unit**  

\[
0 < x < \frac{2}{3}; \quad 0 < y < \frac{2}{3}; \quad 0 < z < \frac{1}{4}; \quad x < \frac{(1+y)2}{2}; \quad y < \min(1-x,(1+x)/2)
\]

**Vertices**  

| 0,0,0 | 1/2,0,0 | 2/3,1/3,0 | 1/3,2/3,0 | 0,1/2,0 |
| 0,0,1/4 | 1/2,0,1/4 | 2/3,1/3,1/4 | 1/3,2/3,1/4 | 0,1/2,1/4 |

**Symmetry Operations**

1. $1$  
2. $3^*$ $0,0,z$  
3. $3$ $0,0,z$  
4. $2$ $x,x,\frac{1}{4}$  
5. $2$ $x,2x,\frac{1}{4}$  
6. $2$ $2x,\frac{1}{4}$  
7. $\bar{1}$ $0,0,0$  
8. $\bar{3}^*$ $0,0,z; 0,0,0$  
9. $\bar{3}$ $0,0,z; 0,0,0$  
10. $c (0,0,1/2)$ $x,0,z$  
11. $c (0,0,1/2)$ $x,0,z$  
12. $c (0,0,1/2)$ $0,y,z$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

## Positions

<table>
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<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>i</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>h .2</td>
<td>[v, u, 0]</td>
</tr>
<tr>
<td>6</td>
<td>g 1</td>
<td>[v, u, w]</td>
</tr>
<tr>
<td>4</td>
<td>f 3..</td>
<td>0,0,w</td>
</tr>
<tr>
<td>4</td>
<td>e 3..</td>
<td>0,0,z</td>
</tr>
<tr>
<td>2</td>
<td>d 3.2</td>
<td>2/3,1/3,1/4</td>
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<tr>
<td>2</td>
<td>c 3.2</td>
<td>1/3,2/3,1/4</td>
</tr>
<tr>
<td>2</td>
<td>b 3..</td>
<td>0,0,0</td>
</tr>
<tr>
<td>2</td>
<td>a 3.2</td>
<td>0,0,1/4</td>
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## Coordinates

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<tr>
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<td>i</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td>6</td>
<td>h .2</td>
<td>(2) y,x,y,z [v,u,w]</td>
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<tr>
<td>6</td>
<td>g 1</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<td>f 3..</td>
<td>(4) x,y,z [v,u,w]</td>
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<tr>
<td>4</td>
<td>e 3..</td>
<td>(5) x+y,y,z [u+v,w]</td>
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<td>(6) x,x-y,z [v,u-w]</td>
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<td>c 3.2</td>
<td>(7) x,y,z [v,u,w]</td>
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<tr>
<td>2</td>
<td>b 3..</td>
<td>(8) x,y,z [v,u-w]</td>
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<tr>
<td>2</td>
<td>a 3.2</td>
<td>(9) x,y,z [v,u-w]</td>
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</tbody>
</table>

## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along [0,0,1]</th>
<th>Along [1,0,0]</th>
<th>Along [2,1,0]</th>
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</thead>
<tbody>
<tr>
<td>p6</td>
<td>m</td>
<td>m</td>
<td>p2</td>
</tr>
<tr>
<td>a* = a</td>
<td>a* = c</td>
<td>a* = c/2</td>
<td>a* = c/2</td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = (a + 2b)/2</td>
<td>b* = b/2</td>
<td>b* = b/2</td>
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<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,1/4</td>
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</tr>
</tbody>
</table>
Origin at center (3 1') at 3 1c1'

Asymmetric unit 0 \leq x \leq 2/3; 0 \leq y \leq 2/3; 0 \leq z \leq 1/4; x \leq (1+y)/2; y \leq \min(1-x,(1+x)/2)

Vertices 0,0,0 1/2,0,0 2/3,1/3,0 1/3,2/3,0 0,1/2,0 0,0,1/4 1/2,0,1/4 2/3,1/3,1/4 1/3,2/3,1/4 0,1/2,1/4

Symmetry Operations

For 1 + set

(1) 1 (1 0,0,0) (2) 3' 0,0,z (3z 0,0,0) (3) 3' 0,0,z (3z' 0,0,0)
(4) 2 x,x,1/4 (2z 0,0,1/2) (5) 2 x,2x,1/4 (2z 0,0,1/2) (6) 2 2x,x,1/4 (2z 0,0,1/2)
(7) 1 (1 0,0,0) (8) 3' 0,0,z; 0,0,0 (3z 0,0,0) (9) 3' 0,0,z; 0,0,0 (3z' 0,0,0)
(10) c (0,0,1/2) x,x,z (m3 0,0,1/2) (11) c (0,0,1/2) x,0,z (m3 0,0,1/2) (12) c (0,0,1/2) 0,y,z (m1 0,0,1/2)
For $1'$ + set

(1) $1'$
   $(1|0,0,0)'$

(2) $3'$
   $0,0,z$
   $(3_2|0,0,0)'$

(3) $3'$
   $0,0,z$
   $(3_z|0,0,0)'$

(4) $2'$
   $x,x,1/4$
   $(2_z|0,0,1/2)'$

(5) $2'$
   $x,2x,1/4$
   $(2_z|0,0,1/2)'$

(6) $2'$
   $2x,x,1/4$
   $(2_z|0,0,1/2)'$

(7) $\bar{1}'$
   $(\bar{1}|0,0,0)'

(8) $3'$
   $0,0,z$
   $0,0,0$
   $(3_z|0,0,0)'$

(9) $3'$
   $0,0,z$
   $0,0,0$
   $(3_z|0,0,0)'$

(10) $c'$
    $(0,0,1/2)$
    $x,x,z$
    $(m_3|0,0,1/2)'$

(11) $c'$
    $(0,0,1/2)$
    $x,0,z$
    $(m_2|0,0,1/2)'$

(12) $c'$
    $(0,0,1/2)$
    $0,y,z$
    $(m_1|0,0,1/2)'$

Generators selected
(1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); $1'$.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
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<tr>
<th>Multiplicity</th>
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<tr>
<td>12</td>
<td>$i$</td>
<td>$11'$</td>
</tr>
<tr>
<td>12 i</td>
<td>$1$</td>
<td>$x,y,z [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td>$(1</td>
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Symmetry of Special Projections

Along $[0,0,1]$  
$a^* = a$  
$b^* = b$
Origin at $0,0,z$

Along $[1,0,0]$  
$a^* = c$  
$b^* = (a + 2b)/2$
Origin at $x,0,0$

Along $[2,1,0]$  
$a^* = c/2$  
$b^* = b/2$
Origin at $x,x/2,0$
Origin at center \(3'c\) at \(3'1c\)

**Asymmetric unit**

\[
\begin{align*}
\text{Vertices} & : \quad 0,0,0 ; \quad 1/2,0,0 ; \quad 2/3,1/3,0 ; \quad 1/3,2/3,0 ; \quad 0,1/2,0 ; \\
 & \quad 0,0,1/4 ; \quad 1/2,0,1/4 ; \quad 2/3,1/3,1/4 ; \quad 1/3,2/3,1/4 ; \quad 0,1/2,1/4 \\
\text{Symmetry Operations} & : \\
(1) & : 1 \\
(2) & : 3^+ \text{ c}(0,0,z) \quad (3) & : 3^- \text{ c}(0,0,z) \\
(4) & : 2' \text{ c}(x,x,1/4) \quad (5) & : 2' \text{ c}(x,2x,1/4) \quad (6) & : 2' \text{ c}(2x,x,1/4) \\
(7) & : 1' \text{ c}(0,0,0)' \quad (8) & : 3'' \text{ c}(0,0,0)' \quad (9) & : 3'' \text{ c}(0,0,0)' \\
(10) & : c(0,0,1/2) \text{ c}(x,z) \quad (11) & : c(0,0,1/2) \text{ c}(0,0,z) \quad (12) & : c(0,0,1/2) \text{ c}(0,y,z) \\
(\text{m}_3 & : 0,0,1/2) \quad (\text{m}_2 & : 0,0,1/2) \quad (\text{m}_1 & : 0,0,1/2)
\end{align*}
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<tr>
<th>No.</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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<tr>
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<td>.2'</td>
<td>x,x,1/4 [u,u,w] x,2x,1/4 [u,0,w] 2x,x,1/4 [0,u,w]</td>
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<td>1'</td>
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<td>3..</td>
<td>1/3,2/3,z [0,0,w] 1/3,2/3,z+1/2 [0,0,w] 2/3,1/3,z [0,0,w] 2/3,1/3,z+1/2 [0,0,w]</td>
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<td>3..</td>
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<td>3.2'</td>
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Symmetry of Special Projections

Along [0,0,1] p6mm Along [1,0,0] p2mg Along [2,1,0] P2\(\text{a}_1\) 211
\(a^* = a \quad b^* = b\) \(a^* = c \quad b^* = (a + 2b)/2\) \(a^* = c/2 \quad b^* = b/2\)
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
Origin at center (3'') at $\bar{3}'1c'$

Asymmetric unit

\begin{align*}
0 \leq x & \leq 2/3; & 0 \leq y & \leq 2/3; & 0 \leq z & \leq 1/4; & x & \leq (1+y)/2; & y & \leq \min(1-x, (1+x)/2) \\
\end{align*}

Vertices

\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/3,2/3,0 & & 0,1/2,0 \\
0,0,1/4 & & 1/2,0,1/4 & & 2/3,1/3,1/4 & & 1/3,2/3,1/4 & & 0,1/2,1/4 \\
\end{align*}

Symmetry Operations

\begin{align*}
(1) & & 1 & & 1 & & 0,0,0 & & (1) & & 0,0,0 & & (1) & & 0,0,0 & \\
(2) & & 3' & & 0,0,z & & (3_z) & & 0,0,0 & & (3) & & 0,0,z & & (3_z) & & 0,0,0 & \\
(3) & & 3' & & 0,0,z & & (3_z) & & 0,0,0 & & (3) & & 0,0,z & & (3_z) & & 0,0,0 & \\
(4) & & 2 & & x,x,1/4 & & (2_z) & & 1/2,0,1/2 & & (2) & & x,x,1/4 & & (2_z) & & 1/2,0,1/2 & \\
(5) & & 2 & & x,2x,1/4 & & (2_z) & & 2/3,1/3,1/4 & & (2) & & x,2x,1/4 & & (2_z) & & 2/3,1/3,1/4 & \\
(6) & & 2 & & 2x,x,1/4 & & (2_z) & & 2/3,1/3,1/4 & & (2) & & 2x,x,1/4 & & (2_z) & & 2/3,1/3,1/4 & \\
(7) & & \bar{1}' & & 0,0,0 & & (1) & & 0,0,0 & & (1) & & 0,0,0 & & (1) & & 0,0,0 & \\
(8) & & 3'' & & 0,0,z & & (3_z) & & 0,0,0 & & (3) & & 0,0,z & & (3_z) & & 0,0,0 & \\
(9) & & 3'' & & 0,0,z & & (3_z) & & 0,0,0 & & (3) & & 0,0,z & & (3_z) & & 0,0,0 & \\
(10) & & c' & & (0,0,1/2) & & x,x,z & & (m_3) & & (0,0,1/2) & & (m_3) & & (0,0,1/2) & & (m_3) & & (0,0,1/2) & \\
(11) & & c' & & (0,0,1/2) & & x,0,z & & (m_3) & & (0,0,1/2) & & (m_3) & & (0,0,1/2) & & (m_3) & & (0,0,1/2) & \\
(12) & & c' & & (0,0,1/2) & & 0,y,z & & (m_3) & & (0,0,1/2) & & (m_3) & & (0,0,1/2) & & (m_3) & & (0,0,1/2) & \\
\end{align*}
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

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Symmetry of Special Projections

Along [0,0,1] p6m'm'
- a* = a  b* = b
- Origin at 0,0,z

Along [1,0,0] p2m'g'
- a* = c  b* = (a + 2b)/2
- Origin at 0,0,1/2

Along [2,1,0] p 211
- a* = c/2  b* = b/2
- Origin at x,x/2,0
Origin at center \((3)\) at \(\text{3} \text{1c}'\)

**Asymmetric unit**  
\[0 \leq x \leq 2/3;\quad 0 \leq y \leq 2/3;\quad 0 \leq z \leq 1/4;\quad x \leq (1+y)/2;\quad y \leq \min(1-x,(1+x)/2)\]

**Vertices**  
0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0
0,0,1/4 \quad 1/2,0,1/4 \quad 2/3,1/3,1/4 \quad 1/3,2/3,1/4 \quad 0,1/2,1/4

**Symmetry Operations**

1. \((1)\) 1
   
2. \((2)\) 3* \((0,0,z)\)
   
3. \((3)\) 3* \((0,0,z)\)

4. \((4)\) 2' \(x,x,1/4\)
   
5. \((5)\) 2' \(x,2x,1/4\)
   
6. \((6)\) 2' \(x,1/2,x\)

7. \((7)\) \(\overline{1}\) \((0,0,0)\)

8. \((8)\) \(3'\) \((0,0,z;0,0,0)\)

9. \((9)\) \(\overline{3}'\) \((0,0,z;0,0,0)\)

10. \((10)\) \(c'\) \((0,0,1/2)\) \(x,x,z\)

11. \((11)\) \(c'\) \((0,0,1/2)\) \(x,0,z\)

12. \((12)\) \(c'\) \((0,0,1/2)\) \(0,y,z\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

12  
Position   

<p>| | | | | | | |</p>
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<tr>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>i</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) (y, \bar{x}, \bar{y}, z [\bar{v}, \bar{u}, w])</td>
<td>(3) (\bar{x} + y, \bar{x}, z [\bar{u} + v, \bar{u}, w])</td>
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<tr>
<td></td>
<td></td>
<td>(4) (\bar{y}, x, z + 1/2 [v,u,w])</td>
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<td>(5) (x + y, y, z + 1/2 [u-v, \bar{v}, w])</td>
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<td></td>
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<td>(7) (x, y, z [u,v,w])</td>
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<td>(9) (x-y, x-z [u+v, u, w])</td>
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<td></td>
<td>(10) (y, x+z+1/2 [v,u,w])</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(11) (x-y, y, z+1/2 [u-v, \bar{v}, w])</td>
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6  
Position   

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<tbody>
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<td>h</td>
<td>2'</td>
<td>x, 1/4 [u,u,w]</td>
<td>x,2x,1/4 [(\bar{u}, 0, w)]</td>
<td>2x, x,1/4 [0, u,w]</td>
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<tr>
<td></td>
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<td></td>
<td>x, 3/4 [u,u,w]</td>
<td>x,2x,3/4 [(\bar{u}, 0, w)]</td>
<td>2x, x,3/4 [0, u,w]</td>
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<tr>
<td>6</td>
<td>g</td>
<td>\bar{1}</td>
<td>1/2,0,0 [u,v,w]</td>
<td>0,1/2,0 [(\bar{v}, u-v, w)]</td>
<td>1/2, 1/2, 0 [(\bar{u}+v, \bar{u}, w)]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>0,1/2,1/2 [v,u,w]</td>
<td>1/2,0,1/2 [u-v, (\bar{v}, w)]</td>
<td>1/2, 1/2, 1/2 [(\bar{u}, \bar{u}+v, w)]</td>
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4  
Position   

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<td>f</td>
<td>3..</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>1/3,2/3, z + 1/2 [0,0,w]</td>
<td>2/3,1/3, z [0,0,w]</td>
<td>2/3,1/3, z+1/2 [0,0,w]</td>
</tr>
<tr>
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<td></td>
<td></td>
<td>0,0,z [0,0,w]</td>
<td>0,0, z+1/2 [0,0,w]</td>
<td>0,0, z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
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2  
Position   

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<td>d</td>
<td>3.2'</td>
<td>2/3,1/3,1/4 [0,0,w]</td>
<td>1/3,2/3,3/4 [0,0,w]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>1/3,2/3,1/4 [0,0,w]</td>
<td>1/3,2/3,3/4 [0,0,w]</td>
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1  
Position   

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</thead>
<tbody>
<tr>
<td>1</td>
<td>b</td>
<td>\bar{3}..</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
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</tr>
<tr>
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<td></td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
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</table>

Symmetry of Special Projections

Along [0,0,1]  
p6'mmm'

\(a^* = a\), \(b^* = b\)

Origin at 0,0,z

Along [1,0,0]  
p2'mg'

\(a^* = c\), \(b^* = (a + 2b)/2\)

Origin at x,0,0

Along [2,1,0]  
p 2'11

\(a^* = c/2\), \(b^* = b/2\)

Origin at x,x/2,0
**Origin** on center ($\overline{3}m1$)

**Asymmetric unit**

<table>
<thead>
<tr>
<th>$0 \leq x &lt; 2/3$;</th>
<th>$0 \leq y &lt; 1/3$;</th>
<th>$0 \leq z &lt; 1$;</th>
<th>$x &lt; (1+y)/2$;</th>
<th>$y &lt; x/2$</th>
</tr>
</thead>
</table>

**Vertices**

<table>
<thead>
<tr>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>2/3,1/3,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,1</td>
<td>1/2,0,1</td>
<td>2/3,1/3,1</td>
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</tbody>
</table>

**Symmetry Operations**

<table>
<thead>
<tr>
<th>(1) 1</th>
<th>(2) $3^+ 0,0,z$</th>
<th>(3) $3^- 0,0,z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1</td>
<td>0,0,0)</td>
<td>$(3_z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) 2</th>
<th>(5) 2</th>
<th>(6) 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x,0</td>
<td>x,0,0</td>
<td>0,y,0</td>
</tr>
<tr>
<td>$(2_x</td>
<td>0,0,0)$</td>
<td>$(2_z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) $\overline{1}$</th>
<th>(8) $\overline{3}^+ 0,0,z; 0,0,0$</th>
<th>(9) $\overline{3}^- 0,0,z; 0,0,0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1</td>
<td>0,0,0)$</td>
<td>$(3_z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) m</th>
<th>(11) m</th>
<th>(12) m</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x,z</td>
<td>x,2x,z</td>
<td>2x,x,z</td>
</tr>
<tr>
<td>$(m_x</td>
<td>0,0,0)$</td>
<td>$(m_x</td>
</tr>
</tbody>
</table>
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positions</td>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
</tr>
<tr>
<td>12 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) -y,x,z [v,u,w]</td>
</tr>
<tr>
<td>6 i .m.</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>6 h .2</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>6 g .2</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>3 f .2/m</td>
<td>1/2,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>3 e .2/m</td>
<td>1/2,0,0 [u,0,0]</td>
</tr>
<tr>
<td>2 d 3m</td>
<td>1/3,2/3,2z [0,0,0]</td>
</tr>
<tr>
<td>2 c 3m</td>
<td>0,0,2z [0,0,0]</td>
</tr>
<tr>
<td>1 b 3m</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a 3m</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p6'mm'  
  \( a^* = a \ b^* = b \)
- Along [1,0,0] p2111'  
  \( a^* = c \ b^* = (a + 2b)/2 \)
- Along [2,1,0] p2'mm'  
  \( a^* = b/2 \ b^* = c \)

Origin at 0,0,0
Origin on center (3\textsuperscript{m11}')

Asymmetric unit

\begin{align*}
0 \leq x & \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2 \\
0,0,0 & \quad 1/2,0,0 \quad 2/3,1/3,0 \\
0,0,1 & \quad 1/2,0,1 \quad 2/3,1/3,1
\end{align*}

Symmetry Operations

For 1 + set

\begin{align*}
(1) & \quad 1 \\
(1') & \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(2_3) & \quad 0,0,0 \\
(3) & \quad 3' \quad 0,0,z \\
(3') & \quad 0,0,0 \\
(4) & \quad 2 \quad x,x,0 \\
(2_x) & \quad 0,0,0 \\
(5) & \quad 2 \quad x,0,0 \\
(2_z) & \quad 0,0,0 \\
(6) & \quad 2 \quad 0,y,0 \\
(2_y) & \quad 0,0,0 \\
(7) & \quad 1 \quad 0,0,0 \\
(1') & \quad 0,0,0 \\
(8) & \quad 3 \quad 0,0,z; 0,0,0 \\
(3_x) & \quad 0,0,0 \\
(9) & \quad 3' \quad 0,0,z; 0,0,0 \\
(3_z') & \quad 0,0,0 \\
(10) & \quad m \quad x,x,z \\
(m_x) & \quad 0,0,0 \\
(11) & \quad m \quad x,2x,z \\
(m_y) & \quad 0,0,0 \\
(12) & \quad m \quad 2x,x,z \\
(m_y) & \quad 0,0,0
\end{align*}
For 1' + set

(1) 1'  
   (1 | 0,0,0)'
(2) 3'  
   (3 | 0,0,0)'
(3) 3'  
   (3 | 1 | 0,0,0)'
(4) 2'  
   (2 | x,x,0)
   (2 | y,0,0,0)'
(5) 2'  
   (2 | x,0,0)
   (2 | y,0,0,0)'
(6) 2'  
   (2 | y,0,0)
(7) 1'  
   (1 | 0,0,0)'
(8) 3'  
   (3 | 0,0,0)'
(9) 3'  
   (3 | 1 | 0,0,0)'
(10) m'  
     (m | x,x,z)
     (m | x,0,0,0)'
(11) m'  
     (m | x,2x,z)
     (m | x,0,0,0)'
(12) m'  
     (m | 2x,x,z)
     (m | x,0,0,0)'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
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<td>x,y,z</td>
<td>[0,0,0]</td>
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<td>y,x-y,z</td>
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<td>x+y,x,z</td>
<td>[0,0,0]</td>
<td>(3)</td>
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<tr>
<td></td>
<td>x,y,z</td>
<td>[0,0,0]</td>
<td>(4)</td>
</tr>
<tr>
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<td>x-y,y,z</td>
<td>[0,0,0]</td>
<td>(5)</td>
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<td>x-y,x,z</td>
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<td>(6)</td>
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<td>y,x+y,z</td>
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<td>y,x+y,z</td>
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<td>x,x,z</td>
<td>[0,0,0]</td>
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<td>x,x,z</td>
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<td>x,0,1/2</td>
<td>[0,0,0]</td>
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<td>x,0,1/2</td>
<td>[0,0,0]</td>
<td>(20)</td>
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<td>6 g .2.1'</td>
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<td>3 f .2/m.1'</td>
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<td>[0,0,0]</td>
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<tr>
<td>2 d 3m.1'</td>
<td>1/3,2/3,z</td>
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<tr>
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<td>2/3,1/3,z</td>
<td>[0,0,0]</td>
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<tr>
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<td>[0,0,0]</td>
<td>(35)</td>
</tr>
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<td></td>
<td>0,0,z</td>
<td>[0,0,0]</td>
<td>(36)</td>
</tr>
<tr>
<td>1 b 3m.1'</td>
<td>0,0,1/2</td>
<td>[0,0,0]</td>
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<tr>
<td>1 a 3m.1'</td>
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<td>[0,0,0]</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Formula</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p6mm1'</td>
<td>$a^* = a$</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b$</td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p211'</td>
<td>$a^* = c$</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = (a+2b)/2$</td>
<td></td>
</tr>
<tr>
<td>Along [2,1,0]</td>
<td>p2mm1'</td>
<td>$a^* = c$</td>
<td>Origin at x,x/2,0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$b^* = b/2$</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on center (3’m1)

**Asymmetric unit**

\[0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2\]

**Vertices**

- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 0,0,1
- 1/2,0,1
- 2/3,1/3,1

**Symmetry Operations**

1. 1
   - \(1\ 0,0,0\)

2. \(3'\ 0,0,z\)
   - \(3_z\ 0,0,0\)

3. \(3'\ 0,0,z\)
   - \(3_z^{-1}\ 0,0,0\)

4. \(2'\ x,x,0\)
   - \((2_x\ 0,0,0)'

5. \(2'\ x,0,0\)
   - \((2_z\ 0,0,0)'

6. \(2'\ 0,y,0\)
   - \((2_y\ 0,0,0)'

7. \(1'\)
   - \((1\ 0,0,0)'

8. \(3'\ 0,0,z; 0,0,0\)
   - \(3_z\ 0,0,0)'

9. \(3'\ 0,0,z; 0,0,0\)
   - \(3_z^{-1}\ 0,0,0)'

10. \(m\ x,x,z\)
    - \(m_{xy}\ 0,0,0\)

11. \(m\ x,2x,z\)
    - \(m_{x} 0,0,0\)

12. \(m\ 2x,x,z\)
    - \(m_{y}\ 0,0,0\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Number</th>
<th>Wyckoff Letter</th>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>j 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>12 j 1 (1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u,v,u,w]</td>
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</tr>
<tr>
<td></td>
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<td>(4) y,x,z [v,u,v,w]</td>
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<td></td>
<td></td>
<td>(5) x-y,y,z [u+v,v,w]</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x+y,z [u,u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(8) y,x+y,z [v-u,v,w]</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(9) x-y,x,z [u-v,u,w]</td>
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<tr>
<td></td>
<td></td>
<td>(10) y,x,z [v,u,v,w]</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(11) x+y,y,z [u-v,u,w]</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(12) x-x,y,z [u,u+v,w]</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>i .m.</td>
<td>x,x,z [u,u,0]</td>
<td>6 i .m. x,x.z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,2x,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,z [u,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>.2'</td>
<td>x,0,1/2 [u,2u,w]</td>
<td>6 h .2' x,0,1/2 [u,2u,w]</td>
</tr>
<tr>
<td></td>
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<td>0,x,1/2 [2u,u,w]</td>
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<tr>
<td></td>
<td></td>
<td>x,x,1/2 [u,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>.2'</td>
<td>x,0,0 [u,2u,w]</td>
<td>6 g .2' x,0,0 [u,2u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,x,0 [2u,u,w]</td>
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</tr>
<tr>
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<td></td>
<td>x,x,0 [u,u,w]</td>
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</tr>
<tr>
<td></td>
<td>.2'/m.</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>3 f .2'/m. 1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
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<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
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<tr>
<td></td>
<td>.2'/m.</td>
<td>1/2,0,0 [0,0,0]</td>
<td>3 e .2'/m. 1/2,0,0 [0,0,0]</td>
</tr>
<tr>
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<td></td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3m.</td>
<td>1/3,2/3,z [0,0,0]</td>
<td>2 d 3m. 1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3m.</td>
<td>0,0,z [0,0,0]</td>
<td>2 c 3m. 0,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3'm.</td>
<td>0,0,1/2 [0,0,0]</td>
<td>1 b 3'm. 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3'm.</td>
<td>0,0,0 [0,0,0]</td>
<td>1 a 3'm. 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p6mm
Along [1,0,0]  p2111'
Along [2,1,0]  p2mm

a* = a  b* = b
a* = c  b* = (a + 2b)/2
Origin at 0,0,z
Origin at x,0,0
Origin at x,x/2,0
Origin on center ($\bar{3}'m'1$)

Asymmetric unit

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0,0,0</th>
<th>0,0,1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1/2,0,0</td>
<td>1/2,0,1</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3,0</td>
<td>2/3,1/3,1</td>
</tr>
</tbody>
</table>

Symmetry Operations

1. $1$

2. $3'$ $0,0,z$
   $(3_z | 0,0,0)$

3. $3'$ $0,0,z$
   $(3_z^{-1} | 0,0,0)$

4. $2$ $x,x,0$
   $(2_{xy} | 0,0,0)$

5. $2$ $x,0,0$
   $(2_x | 0,0,0)$

6. $2$ $0,y,0$
   $(2_y | 0,0,0)$

7. $\bar{1}$
   $(\bar{1} | 0,0,0)$

8. $3''$ $0,0,z; 0,0,0$
   $(3_z | 0,0,0)'$

9. $3''$ $0,0,z; 0,0,0$
   $(3_z^{-1} | 0,0,0)'$

10. $m'$ $x,x,z$
    $(m_{xy} | 0,0,0)'$

11. $m'$ $x,2x,z$
    $(m_x | 0,0,0)'$

12. $m'$ $2x,x,z$
    $(m_y | 0,0,0)'$
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>( (\mathbf{u}, \mathbf{v}, \mathbf{w}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 j 1</td>
<td>(1) ( x, y, z ) [( u, v, w )]</td>
<td>(2) ( y, x-y, z ) [( v-u, v, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) ( x+y, x, z ) [( u+v, u, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) ( y, x ) [( v, u, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) ( x-y, y ) [( u-v, v, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) ( x, x+y ) [( u, u+v, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) ( x, y, z ) [( u, v, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) ( y, x+y, z ) [( v, u+v, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(9) ( x-y, x, z ) [( u-v, u, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) ( y, x, z ) [( v, u, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(11) ( x+y, y, z ) [( u+v, v, w )]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) ( x, x-y, z ) [( u-u, v, w )]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along \([0,0,1] \)**: \( p6m1' \)
  - \( \mathbf{a}^* = \mathbf{a} \)
  - \( \mathbf{b}^* = \mathbf{b} \)
  - Origin at \( 0,0,z \)

- **Along \([1,0,0] \)**: \( p211 \)
  - \( \mathbf{a}^* = \mathbf{c} \)
  - \( \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)
  - Origin at \( 0,0,0 \)

- **Along \([2,1,0] \)**: \( p2m1' \)
  - \( \mathbf{a}^* = \mathbf{c} \)
  - \( \mathbf{b}^* = \mathbf{b}/2 \)
  - Origin at \( x,0,0 \)
Origin on center (3\textsuperscript{m}1)

Asymmetric unit
0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2

Vertices
0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0
0,0,1 \quad 1/2,0,1 \quad 2/3,1/3,1

Symmetry Operations

(1) 1
(1 0,0,0)

(4) 2\textsuperscript{'}, x,0
(2\textsubscript{x},0,0,0)'

(7) 1
(1 0,0,0)

(10) m\textsuperscript{'}, x,x,z
(m\textsubscript{x},0,0,0)'

(2) 3\textsuperscript{*}, 0,0,z
(3\textsubscript{z},0,0,0)

(5) 2\textsuperscript{'}, x,0,0
(2\textsubscript{x},0,0,0)'

(8) 3\textsuperscript{*}, 0,0,z; 0,0,0
(3\textsubscript{z},0,0,0)

(11) m\textsuperscript{'}, x,2x,z
(m\textsubscript{x},0,0,0)'

(3) 3\textsuperscript{*}, 0,0,z
(3\textsubscript{z},0,0,0)

(6) 2\textsuperscript{'}, y,0
(2\textsubscript{y},0,0,0)'

(9) 3\textsuperscript{*}, 0,0,z; 0,0,0
(3\textsubscript{z},0,0,0)

(12) m\textsuperscript{'}, 2x,x,z
(m\textsubscript{y},0,0,0)'}
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).\)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 j 1</td>
<td>((1) \ x,y,z \ [u,v,w]) (\rightarrow (2) \ y,x-y,z \ [v,u,w]) (\rightarrow (3) \ x+y,x,z \ [u+v,u,w]) (\rightarrow (4) \ y,x,z \ [v,u,w]) (\rightarrow (5) \ x,y,z \ [u,u,v,w]) (\rightarrow (6) \ x,y,\bar{z} \ [u,v,u,w]) (\rightarrow (7) \ \bar{x},\bar{y},\bar{z} \ [u,v,w]) (\rightarrow (8) \ \bar{x},\bar{y},z \ [u,v,w]) (\rightarrow (9) \ \bar{x},y,x \ [u,v,u,w]) (\rightarrow (10) \ \bar{y},x,z \ [v,u,w]) (\rightarrow (11) \ \bar{y},x+y,z \ [u+v,u,w]) (\rightarrow (12) \ \bar{x},x-y,z \ [u,u-v,w])</td>
</tr>
<tr>
<td>6 i .m'</td>
<td>(\rightarrow (1) \ x,y,z \ [u,u,w]) (\rightarrow (2) \ x,2x,z \ [u,2u,w]) (\rightarrow (3) \ 2x,2x,z \ [2u,2u,w])</td>
</tr>
<tr>
<td>6 h .2'</td>
<td>(\rightarrow (1) \ x,0,1/2 \ [u,2u,w]) (\rightarrow (2) \ 0,x,1/2 \ [2u,u,w])</td>
</tr>
<tr>
<td>6 g .2'</td>
<td>(\rightarrow (1) \ x,0,1/2 \ [u,2u,w]) (\rightarrow (2) \ 0,x,0 \ [2u,u,w])</td>
</tr>
<tr>
<td>3 f .2'/m'</td>
<td>(\rightarrow (1) \ 1/2,0,1/2 \ [u,2u,w]) (\rightarrow (2) \ 1/2,1/2 \ [2u,u,w])</td>
</tr>
<tr>
<td>3 e .2'/m'</td>
<td>(\rightarrow (1) \ 1/2,0,0 \ [u,2u,w]) (\rightarrow (2) \ 1/2,0 \ [2u,u,w])</td>
</tr>
<tr>
<td>2 d 3m'</td>
<td>(\rightarrow (1) \ 1/3,2/3,z \ [0,0,w]) (\rightarrow (2) \ 2/3,1/3,\bar{z} \ [0,0,w])</td>
</tr>
<tr>
<td>2 c 3m'</td>
<td>(\rightarrow (1) \ 0,0,z \ [0,0,w]) (\rightarrow (2) \ 0,0,\bar{z} \ [0,0,w])</td>
</tr>
<tr>
<td>1 b 3m'</td>
<td>(\rightarrow (1) \ 0,1/2 \ [0,0,w]) (\rightarrow (2) \ 0,0,0 \ [0,0,w])</td>
</tr>
<tr>
<td>1 a 3m'</td>
<td>(\rightarrow (1) \ 0,0,0 \ [0,0,w]) (\rightarrow (2) \ 0,0,0 \ [0,0,w])</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6'm'm</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>(\rightarrow (1) \ x,y,z \ [u,v,w]) (\rightarrow (2) \ y,x-y,z \ [v,u,w]) (\rightarrow (3) \ x+y,x,z \ [u+v,u,w])</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2'11</td>
</tr>
<tr>
<td>(a^* = c)</td>
<td>(b^* = (a + 2b)/2)</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td>(\rightarrow (1) \ x,y,z \ [u,v,w]) (\rightarrow (2) \ y,x-y,z \ [v,u,w]) (\rightarrow (3) \ x+y,x,z \ [u+v,u,w])</td>
</tr>
<tr>
<td>Along [2,1,0]</td>
<td>p2'mm'</td>
</tr>
<tr>
<td>(a^* = c)</td>
<td>(b^* = b/2)</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td>(\rightarrow (1) \ x,y,z \ [u,v,w]) (\rightarrow (2) \ y,x-y,z \ [v,u,w]) (\rightarrow (3) \ x+y,x,z \ [u+v,u,w])</td>
</tr>
</tbody>
</table>
Origin on center \((\overline{3}m1)\)

Asymmetric unit
\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2
\]

Vertices
\[
(0,0,0) \quad (1/2,0,0) \quad (2/3,1/3,0) \\
(0,0,1) \quad (1/2,0,1) \quad (2/3,1/3,1)
\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3 \quad 0,0,z \\
(4) & \quad 2 \quad x,x,0 \\
(5) & \quad 2 \quad x,0,0 \\
(6) & \quad 2 \quad 0,y,0 \\
(7) & \quad \overline{1} \quad \overline{1} \quad 0,0,0 \\
(8) & \quad \overline{3}^* \quad 0,0,z; \quad 0,0,0 \\
(9) & \quad \overline{3} \quad 0,0,z; \quad 0,0,0 \\
(10) & \quad m \quad x,x,z \\
(11) & \quad m \quad x,2x,z \\
(12) & \quad m \quad 2x,x,z
\end{align*}
\]

\[
(\overline{1}) 0,0,0 \\
(\overline{3}) z \quad 0,0,0 \\
(\overline{3}) z^{-1} \quad 0,0,0 \\
(m_x) 0,0,0 \\
(m_x) 0,0,0 \\
(m_y) 0,0,0
\]
For \((0,0,1)\) + set

| (1) \(t' (0,0,1)\) | (2) \(3' (0,0,1)\) & 0,0,z | (3) \(3' (0,0,1)\) & 0,0,z |
|----------------------|-----------------|-----------------|-----------------|
| \((1|0,0,1)\)        | \((3\_|0,0,1)\)' | \((3\_|0,0,1)\)' | \((3\_|0,0,1)\)' |

<table>
<thead>
<tr>
<th>(4) (2' x,x,1/2)</th>
<th>(5) (2' x,0,1/2)</th>
<th>(6) (2' 0,y,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((2,_</td>
<td>0,0,1))'</td>
<td>((2,</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) (\bar{T} 0,0,1/2)</th>
<th>(8) (\bar{T} 0,0,1/2)</th>
<th>(9) (\bar{T} 0,0,1/2)</th>
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<tbody>
<tr>
<td>((\bar{T}</td>
<td>0,0,1))'</td>
<td>((\bar{T}</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) (c' (0,0,1) x,x,z)</th>
<th>(11) (c' (0,0,1) x,2x,z)</th>
<th>(12) (c' (0,0,1) 2x,x,z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((m,_</td>
<td>0,0,1))'</td>
<td>((m,</td>
</tr>
</tbody>
</table>

Generators selected (1); \(t(1,0,0)\); \(t(0,1,0)\); \(t'(0,0,1)\); (2); (4); (7).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0) + ) ((0,0,1)) + ((0,0,1)) + ((0,0,1))</td>
<td>(x,y,z [u,v,w]) (\bar{y},-y,z [\bar{v},u-v,w]) (x+y,x,z [u+\bar{v},\bar{u},w]) (x+y,x,z [u+\bar{v},\bar{u},w])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>((1) x,y,z [u,v,w])</th>
<th>(\bar{y},-y,z [\bar{v},u-v,w])</th>
<th>(x+y,x,z [u+\bar{v},\bar{u},w])</th>
</tr>
</thead>
<tbody>
<tr>
<td>(24 j 1)</td>
<td>(24 i .m.)</td>
<td>(12 h .2')</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(x,x,z [u,u,0])</th>
<th>(x,2x,z [u,0,0])</th>
<th>(2x,x,z [0,0,0])</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\bar{x},\bar{x},z [u,u,0])</td>
<td>(2x,\bar{x},z [0,u,0])</td>
<td>(\bar{x},2\bar{x},z [u,0,0])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(x,0,1/2 [u,2u,w])</th>
<th>(0,x,1/2 [2u,u,w])</th>
<th>(\bar{x},1/2 [u,u,w])</th>
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<tr>
<td>(x,0,1/2 [\bar{u},\bar{2u},w])</td>
<td>(0,\bar{x},1/2 [2u,u,w])</td>
<td>(x,1/2 [u,u,w])</td>
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<tr>
<th>(x,0,0 [u,0,0])</th>
<th>(0,x,0 [0,u,0])</th>
<th>(\bar{x},x,0 [u,0,0])</th>
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<tr>
<td>(\bar{x},0,0 [u,0,0])</td>
<td>(0,\bar{x},0 [0,u,0])</td>
<td>(\bar{x},x,0 [u,\bar{u},0])</td>
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<tr>
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<td>(3m)</td>
<td>(3m)</td>
<td>(3m)</td>
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<td>(0,0,0 [0,0,0])</td>
<td>(0,0,0 [0,0,0])</td>
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</tbody>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p6mm1'</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>( a^* = a )</td>
<td>( b^* = b )</td>
<td></td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p2111'</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>( a^* = c )</td>
<td>( b^* = (a + 2b)/2 )</td>
<td></td>
</tr>
<tr>
<td>[2,1,0]</td>
<td>p_{2a}, 2mm</td>
<td>Origin at x,x/2,1/2</td>
</tr>
<tr>
<td>( a^* = c )</td>
<td>( b^* = b/2 )</td>
<td></td>
</tr>
</tbody>
</table>
Origin on center ($3m'$1)

Asymmetric unit:  
\[ 0 < x < \frac{2}{3}; \quad 0 < y < \frac{1}{3}; \quad 0 < z < 1; \quad x < \frac{(1+y)}{2}; \quad y < \frac{x}{2} \]

Vertices:  
- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $0,0,1$
- $1/2,0,1$
- $2/3,1/3,1$

Symmetry Operations: For $(0,0,0) +$ set

1. $1$
2. $3'$: $0,0,z$  
   $3z|0,0,0$  
3. $3$: $0,0,z$  
   $3z|0,0,0$  
4. $2'$: $x,x,0$  
   $2xy|0,0,0$  
5. $2'$: $x,0,0$  
   $2y|0,0,0$  
6. $1$  
7. $m'$: $x,x,z$  
   $(m_y|0,0,0)'$  
8. $3'$: $0,0,z$  
   $3z|0,0,0$  
9. $3$: $0,0,z$  
   $3z|0,0,0$  
10. $m'$: $x,2x,z$  
    $(m_y|0,0,0)'$  
11. $m'$: $2x,x,z$  
    $(m_y|0,0,0)'$  
12. $m'$: $x,2x,z$  
    $(m_y|0,0,0)'$
For $(0,0,1)' +$ set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>(1) $t'(0,0,1)$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
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<tr>
<td>(2) $3'(0,0,1)$</td>
<td>$(0,0,z)$</td>
</tr>
<tr>
<td>(3) $3'(0,0,1)$</td>
<td>$(0,0,z)$</td>
</tr>
<tr>
<td>(7) $T' 0,0,1/2$</td>
<td>$(3)_z 0,0,1/2$</td>
</tr>
<tr>
<td>(11) $c(0,0,1)$</td>
<td>$x,2x,z$</td>
</tr>
<tr>
<td>(12) $c(0,0,1)$</td>
<td>$2x,x,z$</td>
</tr>
</tbody>
</table>

Generators selected: $(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7)$.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff Letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 $j 1$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
<tr>
<td>$(1) x,y,z \ [u,v,w]$</td>
<td>$(2) \bar{y}, x-y,z \ [\bar{v},u-v,w]$</td>
</tr>
<tr>
<td>$(4) y,x,z \ [v,u,w]$</td>
<td>$(5) x-y,\bar{y},z \ [u+v,v,w]$</td>
</tr>
<tr>
<td>$(7) \bar{x},y,z \ [v,u,w]$</td>
<td>$(8) y,x+y,z \ [v,u-v,w]$</td>
</tr>
<tr>
<td>$(10) \bar{y},x,z \ [\bar{v},u,w]$</td>
<td>$(11) x+y,z \ [u+v,v,w]$</td>
</tr>
<tr>
<td>12 $i .m'$</td>
<td>$x,2x,z \ [u,2u,w]$</td>
</tr>
<tr>
<td>$(\bar{x},x,z \ [\bar{u},u,w])$</td>
<td>$2x,x,z \ [2u,2u,w]$</td>
</tr>
<tr>
<td>12 $h .2$</td>
<td>$x,0,1/2 \ [u,0,0]$</td>
</tr>
<tr>
<td>$(\bar{x},0,1/2 \ [\bar{u},0,0])$</td>
<td>$0,x,1/2 \ [0,u,0]$</td>
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<tr>
<td>12 $g .2'$</td>
<td>$x,0,0 \ [u,2u,w]$</td>
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<tr>
<td>$(\bar{x},0,0 \ [\bar{u},2u,w])$</td>
<td>$0,x,0 \ [2u,\bar{u},w]$</td>
</tr>
<tr>
<td>6 $f .2/m$</td>
<td>$1/2,0,1/2 \ [u,0,0]$</td>
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<tr>
<td>6 $e .2'/m'$</td>
<td>$1/2,0,0 \ [u,2u,w]$</td>
</tr>
<tr>
<td>4 $d 3m'$</td>
<td>$1/3,2/3,0 \ [0,0,w]$</td>
</tr>
<tr>
<td>4 $c 3m'$</td>
<td>$0,0,z \ [0,0,w]$</td>
</tr>
<tr>
<td>2 $b 3m'$</td>
<td>$0,0,1/2 \ [0,0,w]$</td>
</tr>
<tr>
<td>2 $a 3m'$</td>
<td>$0,0,0 \ [0,0,w]$</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] \( \text{p}6\text{mm}1' \)
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
Origin at 0,0,z

Along [1,0,0] \( \text{p}_{2a}^* \text{211} \)
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)
Origin at x,0,1/2

Along [2,1,0] \( \text{p}_{2a}^* \text{2m}^*\text{m}' \)
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)
Origin at x,x/2,1/2
Origin on center (3) at $\overline{3}c1$

Asymmetric unit:

- $0 \leq x \leq 2/3$
- $0 \leq y \leq 2/3$
- $0 \leq z \leq 1/4$
- $x \leq (1+y)/2$
- $y \leq \min(1-x,(1+x)/2)$

Vertices:

- $(0,0,0)$
- $(1/2,0,0)$
- $(2/3,1/3,0)$
- $(1/3,2/3,0)$
- $(0,1/2,0)$
- $(0,0,1/4)$
- $(1/2,0,1/4)$
- $(2/3,1/3,1/4)$
- $(1/3,2/3,1/4)$
- $(0,1/2,1/4)$

Symmetry Operations:

1. $1$
2. $3^+$ $0,0,z$
3. $3^-$ $0,0,z$
4. $2$ $x,x,1/4$
5. $2$ $x,0,1/4$
6. $2$ $0,y,1/4$
7. $\overline{1}$ $(0,0,0)$
8. $\overline{3}^+$ $0,0,z$; $0,0,0$
9. $\overline{3}^-$ $0,0,z$; $0,0,0$
10. $c$ $(0,0,1/2)$ $x,x,z$
11. $c$ $(0,0,1/2)$ $x,2x,z$
12. $c$ $(0,0,1/2)$ $2x,x,z$

165.1.1322 - 1 - 2855
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>12</td>
<td>g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<tr>
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<td>(4) y,x,z+1/2 [v,u,w]</td>
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<tr>
<td></td>
<td></td>
<td>(5) x-y,y,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x,x+y,z+1/2 [u-u+v,w]</td>
</tr>
<tr>
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<td>(7) x,y,z [u,v,w]</td>
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<td>(8) y,x+y,z [v,u-v,w]</td>
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<tr>
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<td>(9) x-y,x,z [u+v,u,w]</td>
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<tr>
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<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
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<tr>
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<td>(11) x+y,y,z+1/2 [u-v,v,w]</td>
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<td>(12) x,x-y,z+1/2 [u-u+v,w]</td>
</tr>
<tr>
<td>6</td>
<td>f .2</td>
<td>x,0,1/4 [u,0,0]</td>
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<tr>
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<td>0,x,1/4 [0,u,0]</td>
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<td>0,x,3/4 [0,u,0]</td>
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<td>x,x,1/4 [u,u,0]</td>
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<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2</td>
<td>a 32</td>
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<tr>
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<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'/*m1'  
Along [1,0,0] p311  
Along [2,1,0] p21m'g  

a* = a   b* = b  
a* = c/2   b* = (a + 2b)/2  
a* = c   b* = b/2  
Origin at 0,0,z  
Origin at x,0,1/4  
Origin at x,x/2,0
**Origin** on center (3 1') at 3c11'

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/4 & \quad 1/2,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/3,2/3,1/4 & \quad 0,1/2,1/4
\end{align*}
\]

**Symmetry Operations**

For 1 + set

\[
\begin{align*}
1 & \quad 3' - & 0,0,z \\
(1) 1 & \quad (3z|0,0,0) & \quad (3z^{-1}|0,0,0) \\
(2) 3' + & \quad 0,0,z \\
(3) 3' - & \quad 0,0,z \\
(4) 2 & \quad x,x,1/4 \\
(2xy|0,0,1/2) & \quad (2x|0,0,1/2) & \quad (2y|0,0,1/2) \\
(5) 2 & \quad x,0,1/4 \\
(2x|0,0,1/2) & \quad (2y|0,0,1/2) \\
(6) 2 & \quad 0,y,1/4 \\
(2z|0,0,1/2) & \quad (2z_{-1}|0,0,1/2) \\
(7) \overline{1} & \quad 3' - & 0,0,z; \quad 0,0,0 \\
(\overline{1}|0,0,0) & \quad (3z|0,0,0) & \quad (3z^{-1}|0,0,0) \\
(8) 3' + & \quad 0,0,z; \quad 0,0,0 \\
(9) \overline{3} & \quad 0,0,z; \quad 0,0,0 \\
(10) c (0,0,1/2) \quad x,x,z \\
(mx|0,0,1/2) & \quad (mx|0,0,1/2) \\
(11) c (0,0,1/2) \quad x,2x,z \\
(mx|0,0,1/2) & \quad (mz|0,0,1/2) \\
(12) c (0,0,1/2) \quad 2x,x,z \\
(mx|0,0,1/2) & \quad (mz|0,0,1/2)
\end{align*}
\]
For $1^\prime +$ set

(1) $1^\prime$
(1 $0,0,0^\prime$

(2) $3^\prime$ 0,0,z
(3 $3^\prime$ 0,0,z

(4) $2^\prime$ x,x,1/4
(2,0,0,0,1/2)$^\prime$

(5) $2^\prime$ x,0,1/4
(2,0,0,0,1/2)$^\prime$

(6) $2^\prime$ 0,y,1/4
(2,0,0,0,1/2)$^\prime$

(7) $1^\prime$
(1 $0,0,0^\prime$

(8) $3^\prime$ 0,0,z; 0,0,0
(3 $3^\prime$ 0,0,z; 0,0,0

(9) $3^\prime$ 0,0,z; 0,0,0
(3 $3^\prime$ 0,0,z; 0,0,0

(10) $c^\prime$ (0,0,1/2) x,x,z
(m,0,0,1/2)$^\prime$

(11) $c^\prime$ (0,0,1/2) x,2x,z
(m,0,0,1/2)$^\prime$

(12) $c^\prime$ (0,0,1/2) 2x,x,z
(m,0,0,1/2)$^\prime$

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); $1^\prime$.

**Positions**

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<th>Site Symmetry</th>
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<td>(1) x,y,z [0,0,0]</td>
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<td>(2) $y^\prime$,x-y,z [0,0,0]</td>
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<td>(3) $x^\prime$+y,x,z [0,0,0]</td>
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<td>(4) y,x,z+1/2 [0,0,0]</td>
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<td>(5) x-y,y,z+1/2 [0,0,0]</td>
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<td>(6) $x^\prime$+y,z+1/2 [0,0,0]</td>
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<td>(8) y,x+y,z [0,0,0]</td>
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<td>(12) $x^\prime$,x,y,z+1/2 [0,0,0]</td>
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<td>6</td>
<td>f .2.1$^\prime$</td>
<td>x,0,1/4 [0,0,0]</td>
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<td>(2) x,0,1/4 [0,0,0]</td>
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<td>(3) $x^\prime$,x,1/4 [0,0,0]</td>
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<td>(4) x,0,3/4 [0,0,0]</td>
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<tr>
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</tr>
<tr>
<td>4</td>
<td>d .3.1$^\prime$</td>
<td>1/3,2,3,z [0,0,0]</td>
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<tr>
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<td>(2) 2/3,1/3,2,3,z+1/2 [0,0,0]</td>
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<td>(3) 2/3,1/3,2,3,z [0,0,0]</td>
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<td>(4) 1/3,2,3,z+1/2 [0,0,0]</td>
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<td>4</td>
<td>c .3.1$^\prime$</td>
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<td>0,0,0 [0,0,0]</td>
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<td>(2) 0,0,1/2 [0,0,0]</td>
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<tr>
<td>2</td>
<td>a 32.1$^\prime$</td>
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</table>

**Symmetry of Special Projections**

Along [0,0,1] p6mm1$^\prime$

Along [1,0,0] p2111$^\prime$

Along [2,1,0] p2mg1$^\prime$

$a^\star = a$ $b^\star = b$

$a^\star = c/2$ $b^\star = (a + 2b)/2$

$a^\star = c$ $b^\star = b/2$

Origin at 0,0,z

Origin at x,0,0

Origin at x,x/2,0
Origin on center (3') at 3’c1

Asymmetric unit

\[
0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{4}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,(1+x)/2)
\]

Vertices

<table>
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<tr>
<th>x</th>
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<th>z</th>
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</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1/4</td>
</tr>
<tr>
<td>1/2</td>
<td>0</td>
<td>0</td>
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<tr>
<td>1/2</td>
<td>0</td>
<td>1/4</td>
</tr>
<tr>
<td>2/3</td>
<td>1/3</td>
<td>0</td>
</tr>
<tr>
<td>1/3</td>
<td>2/3</td>
<td>0</td>
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<tr>
<td>0</td>
<td>1/2</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1/2</td>
<td>1/4</td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 3’ 0,0,z
(3z | 0,0,0)

(3) 3’ 0,0,z
(3z | 0,0,0)

(4) 2’ x,x,1/4
(2xy | 0,0,1/2)'

(5) 2’ x,0,1/4
(2x | 0,0,1/2)'

(6) 2’ y,1/4
(2y | 0,0,1/2)'

(7) 3’ 0,0,0
(1 | 0,0,0)'

(8) 3’ 0,0,0
(3z | 0,0,0)'

(9) 3’ 0,0,0
(3z | 0,0,0)'

(10) c (0,0,1/2) x,x,z
(mxy | 0,0,1/2)

(11) c (0,0,1/2) x,2x,z
(mx | 0,0,1/2)

(12) c (0,0,1/2) 2x,x,z
(my | 0,0,1/2)
**Generators selected**
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>g 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) ( \bar{y},x-y,z ) [v,u-v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(3) ( x+y, \bar{x},z ) [u+v,\bar{u},w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) y,( x),z +1/2 [v,\bar{u},w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) x-y,( \bar{y}),z +1/2 [u+v,v,w]</td>
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<td></td>
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<td>(6) ( x,\bar{x},z ) +1/2 [u-u-v,w]</td>
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<td></td>
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<td>(7) ( \bar{x},y,\bar{z} ) [u,v,w]</td>
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<td></td>
<td></td>
<td>(8) y,( x+y),z [v,u+v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(9) x-y,( x),( \bar{z} ) [u-v,\bar{u},w]</td>
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<td></td>
<td>(10) ( y, \bar{x},z ) +1/2 [v,u,\bar{w}]</td>
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<tr>
<td></td>
<td></td>
<td>(11) ( \bar{y}+y,y,z ) +1/2 [u-v,\bar{v},\bar{w}]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) ( x-x,y,z ) +1/2 [u,\bar{u},v,\bar{w}]</td>
</tr>
</tbody>
</table>

| 6            | f .2'          | \( x,0,1/4 \) [u,2u,w] |
|              |                | \( 0,x,1/4 \) [2u,\bar{u},w] |
|              |                | \( \bar{x},0,3/4 \) [u,2\bar{u},\bar{w}] |
|              |                | \( 0,\bar{x},3/4 \) [2u,u,\bar{w}] |

| 6            | e \( \bar{1}^1 \) | \( 1/2,0,0 \) [0,0,0] |
|              |                | \( 0,1/2,0 \) [0,0,0] |
|              |                | \( 0,1/2,1/2 \) [0,0,0] |
|              |                | \( 1/2,0,1/2 \) [0,0,0] |
|              |                | \( 1/2,1/2,1/2 \) [0,0,0] |

| 4            | d 3.           | \( 1/3,2/3,0 \) [0,0,0] |
|              |                | \( 2/3,1/3,\bar{z} \) +1/2 [0,0,w] |
|              |                | \( 2/3,1/3,\bar{z} \) [0,0,w] |
|              |                | \( 1/3,2/3,\bar{z} \) +1/2 [0,0,\bar{w}] |

| 4            | c 3.           | \( 0,0,0 \) [0,0,0] |
|              |                | \( 0,0,\bar{z} \) [0,0,w] |
|              |                | \( 0,0,\bar{z} \) +1/2 [0,0,\bar{w}] |

| 2            | b \( \bar{3} \) | \( 0,0,0 \) [0,0,0] |
|              |                | \( 0,0,1/2 \) [0,0,0] |

| 2            | a \( 32 \)     | \( 0,0,1/4 \) [0,0,w] |
|              |                | \( 0,0,3/4 \) [0,0,\bar{w}] |

### Symmetry of Special Projections

- **Along [0,0,1]**: p6mm
- **Along [1,0,0]**: \( p_{6mm} \)
- **Along [2,1,0]**: p2mg

<table>
<thead>
<tr>
<th>( \mathbf{a}^* ) = ( \mathbf{a} )</th>
<th>( \mathbf{b}^* ) = ( \mathbf{b} )</th>
<th>( \mathbf{a}^* = c/2 )</th>
<th>( \mathbf{b}^* = (a+2b)/2 )</th>
<th>( \mathbf{a}^* = c )</th>
<th>( \mathbf{b}^* = b/2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>
**Origin** on center (3') at 3'c'1

**Asymmetric unit**

\[
\begin{align*}
0 & \leq x \leq 2/3; \\
0 & \leq y \leq 2/3; \\
0 & \leq z \leq 1/4; \\
x & \leq (1+y)/2; \\
y & \leq \min(1-x,(1+x)/2)
\end{align*}
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 \quad 2/3,1/3,0 \\
0,0,1/4 & \quad 1/2,0,1/4 \quad 2/3,1/3,1/4
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3' \quad 0,0,z \\
(3) & \quad 3' \quad 0,0,z \quad (3_z,0,0,0)
\end{align*}
\]

\[
\begin{align*}
(4) & \quad 2 \quad x,x,1/4 \\
(5) & \quad 2 \quad x,0,1/4 \\
(6) & \quad 2 \quad 0,y,1/4
\end{align*}
\]

\[
\begin{align*}
(7) & \quad 1' \quad (3_z,0,0,0) \\
(8) & \quad 3' \quad 0,0,z; 0,0,0 \\
(9) & \quad 3' \quad 0,0,z; 0,0,0
\end{align*}
\]

\[
\begin{align*}
(10) & \quad c' \quad (0,0,1/2) \quad x,x,z \\
(11) & \quad c' \quad (0,0,1/2) \quad x,2x,z \\
(12) & \quad c' \quad (0,0,1/2) \quad 2x,x,z
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

## Positions

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<tbody>
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<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td>(4) y,x,z+1/2 [v,u,w]</td>
<td>(3) x+y,x,z [u+v,u-w]</td>
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<tr>
<td>(7) x,y,z [u,v,w]</td>
<td>(6) x,x+y,z+1/2 [u,u+v,w]</td>
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<tr>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td>(9) x,y,x,z [u-v,u,w]</td>
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<tr>
<td>6 f 0.2 x,0,1/4 [u,0,0]</td>
<td>0,x,1/4 [0,u,0]</td>
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<tr>
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<td>x,x,1/4 [u,u,0]</td>
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<tr>
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<td>0,x,3/4 [0,u,0]</td>
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<tr>
<td>6 e 1/1 1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
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<tr>
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<td>2/3,1/3,z+1/2 [0,0,w]</td>
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<td>0,0,z [0,0,w]</td>
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<td>0,0,z+1/2 [0,0,w]</td>
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<td>2 b 3.. 0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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<td>2 a 32. 0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

## Symmetry of Special Projections

Along [0,0,1]  p6m'm'  
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0]  p2'11  
\[ a^* = c/2 \quad b^* = (a + 2b)/2 \]
Origin at x,0,0

Along [2,1,0]  p2m'g'  
\[ a^* = c \quad b^* = b/2 \]
Origin at x,x/2,0
**Origin** on center (3) at 3c'1

**Asymmetric unit**
- \(0 \leq x \leq 2/3;\)
- \(0 \leq y \leq 2/3;\)
- \(0 \leq z \leq 1/4;\)
- \(x \leq (1+y)/2;\)
- \(y \leq \text{min}(1-x,(1+x)/2)\)

**Vertices**
- \((0,0,0)\)
- \((1/2,0,0)\)
- \((2/3,1/3,0)\)
- \((1/3,2/3,0)\)
- \((0,1/2,0)\)
- \((0,0,1/4)\)
- \((1/2,0,1/4)\)
- \((2/3,1/3,1/4)\)
- \((1/3,2/3,1/4)\)
- \((0,1/2,1/4)\)

**Symmetry Operations**

(1) 1
(2) \(3^+ (0,0,z)\)
(3) \(3^- (0,0,z)\)
(4) \(2' x,x,1/4\)
(5) \(2' x,0,1/4\)
(6) \(2' 0,y,1/4\)
(7) \(\overline{1}(0,0,0)\)
(8) \(\overline{3}^- (0,0,z; 0,0,0)\)
(9) \(\overline{3}^+ (0,0,z; 0,0,0)\)
(10) \(c' (0,0,1/2) x,x,z\)
(11) \(c' (0,0,1/2) x,2x,z\)
(12) \(c' (0,0,1/2) 2x,x,z\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<td>(5) x-y,y,z+1/2 [u+v,w]</td>
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<td>(7) x,y,z [u,v,w]</td>
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<td>0,0,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6"m'm' Along [1,0,0] p2'11 Along [2,1,0] p2'mg'

a* = a   b* = b   a* = c/2   b* = (a + 2b)/2   a* = c   b* = b/2

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
Origin on center (3m)

Asymmetric unit  
\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{6}; \quad x \leq \frac{y}{2}; \quad y \leq \min(1-x, 2x) \]

Vertices  
\[ (0, 0, 0) \quad 2/3, 1/3, 0 \quad 1/3, 2/3, 0 \]
\[ (0, 0, 1/6) \quad 2/3, 1/3, 1/6 \quad 1/3, 2/3, 1/6 \]
Symmetry Operations

For $(0,0,0) +$ set

(1) 1
(2) $3^+$ 0,0,z
(3) $3^-$ 0,0,z
(4) $2^\times$ x,x,0
(5) 2 x,0,0
(6) 2 0,y,0
(7) $\bar{T}$
(8) $3^+$ 0,0,z; 0,0,0
(9) $3^-$ 0,0,z; 0,0,0
(10) m x,$\bar{x}$,z
(11) m x,2x,z
(12) m 2x,x,z

For $(2/3,1/3,1/3) +$ set

(1) t (2/3,1/3,1/3)
(2) $3^+$ (0,0,1/3) 1/3,1/3,z
(3) $3^-$ (0,0,1/3) 1/3,0,z
(4) $2^\times$ x-1/6,1/6
(5) 2 (1/2,0,0) x,1/6,1/6
(6) 2 1/3,y,1/6
(7) $\bar{T}$
(8) $3^+$ 1/3,-1/3,z; 1/3,-1/3,1/3
(9) $3^-$ 1/3,2/3,z; 1/3,2/3,1/3
(10) g (1/6,-1/6,1/3)
(11) g (1/6,1/3,1/3)
(12) g (2/3,1/3,1/3)

For $(1/3,2/3,2/3) +$ set

(1) t (1/3,2/3,2/3)
(2) $3^+$ (0,0,2/3) 0,1/3,z
(3) $3^-$ (0,0,2/3) 1/3,1/3,z
(4) $2^\times$ x+1/6,1/6
(5) 2 x,1/3,1/3
(6) 2 (0,1/2,0) 1/6,y,1/3
(7) $\bar{T}$
(8) $3^+$ 2/3,1/3,z; 2/3,1/3,1/3
(9) $3^-$ -1/3,1/3,z; -1/3,1/3,1/3
(10) g (-1/6,1/6,2/3)
(11) g (1/3,2/3,2/3)
(12) g (1/3,1/6,2/3)

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +

166.1.1327 - 3 - 2867
Symmetry of Special Projections

Along [0,0,1] p6'mm'  
\( \mathbf{a}^* = \frac{2\mathbf{a} + \mathbf{b}}{3} \)  \( \mathbf{b}^* = \frac{-\mathbf{a} + \mathbf{b}}{3} \)  
Origin at 0,0,z

Along [1,0,0] p2111'  
\( \mathbf{a}^* = \frac{-\mathbf{a} - 2\mathbf{b} + \mathbf{c}}{3} \)  \( \mathbf{b}^* = \frac{\mathbf{a} + 2\mathbf{b}}{2} \)  
Origin at x,0,0

Along [2,1,0] p2mm'  
\( \mathbf{a}^* = \frac{\mathbf{b}}{2} \)  \( \mathbf{b}^* = \frac{\mathbf{c}}{3} \)  
Origin at x,x/2,0
R3m1'  
166.2.1328  

3m1'  
R32/m1'  

Trigonal
Origin on center (\(\overline{3}m1'\))

Asymmetric unit: 
- \(0 \leq x \leq 2/3;\) 
- \(0 \leq y \leq 2/3;\) 
- \(0 \leq z \leq 1/6;\) 
- \(x \leq y/2;\) 
- \(y \leq \min(1-x,2x)\)

Vertices: 
- \(0,0,0\) 
- \(2/3,1/3,0\) 
- \(1/3,2/3,0\) 
- \(0,0,1/6\) 
- \(2/3,1/3,1/6\) 
- \(1/3,2/3,1/6\)
**Symmetry Operations**

For (0,0,0) + set

<table>
<thead>
<tr>
<th>(1) 1</th>
<th>(2) (3^+ \ 0,0,z)</th>
<th>(3) (3^- \ 0,0,z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) [0,0,0]</td>
<td>(3z</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) 2</th>
<th>(5) 2 (x,0,0)</th>
<th>(6) 2 (0,y,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2(x)</td>
<td>0,0,0)</td>
<td>(2(z)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) (\bar{T})</th>
<th>(8) (3^+ \ 0,0,z; 0,0,0)</th>
<th>(9) (3^- \ 0,0,z; 0,0,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{T})</td>
<td>0,0,0)</td>
<td>(3z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) m (x,\bar{x},z)</th>
<th>(11) m (x,2x,z)</th>
<th>(12) m (2x,x,z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m(x)</td>
<td>0,0,0)</td>
<td>(m(x)</td>
</tr>
</tbody>
</table>

For (2/3,1/3,1/3) + set

<table>
<thead>
<tr>
<th>(1) t</th>
<th>(2) (3^+ \ (0,0,1/3))</th>
<th>(3) (3^- \ (0,0,1/3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1/2,1/3,1/3)</td>
<td>(1/2,1/3,1/3)</td>
<td>(1/2,1/3,1/3)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) 2</th>
<th>(5) 2 (x,1/6,1/6)</th>
<th>(6) 2 (1/3,y,1/6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2(x)</td>
<td>2/3,1/3,1/3)</td>
<td>(2(z)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) (\bar{T})</th>
<th>(8) (3^+ \ 1/3,-1/3,z; 1/3,-1/3,1/3)</th>
<th>(9) (3^- \ 1/3,2/3,z; 1/3,2/3,1/3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{T})</td>
<td>2/3,1/3,1/3)</td>
<td>(3z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) g</th>
<th>(11) g (1/6,1/3,1/3)</th>
<th>(12) g (2/3,1/3,1/3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m(x)</td>
<td>2/3,1/3,1/3)</td>
<td>(m(x)</td>
</tr>
</tbody>
</table>

For (1/3,2/3,2/3) + set

<table>
<thead>
<tr>
<th>(1) t</th>
<th>(2) (3^+ \ (0,0,2/3))</th>
<th>(3) (3^- \ (0,0,2/3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1/2,3/2,2/3)</td>
<td>(1/2,3/2,2/3)</td>
<td>(1/2,3/2,2/3)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) 2</th>
<th>(5) 2 (x,1/6,1/6)</th>
<th>(6) 2 (0,1/2,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2(x)</td>
<td>1/3,2/3,2/3)</td>
<td>(2(z)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) (\bar{T})</th>
<th>(8) (3^+ \ 2/3,1/3,z; 2/3,1/3,1/3)</th>
<th>(9) (3^- \ -1/3,1/3,z; -1/3,1/3,1/3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{T})</td>
<td>1/3,2/3,2/3)</td>
<td>(3z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) g</th>
<th>(11) g (1/6,1/3,1/3)</th>
<th>(12) g (2/3,1/3,1/3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m(x)</td>
<td>1/3,2/3,2/3)</td>
<td>(m(x)</td>
</tr>
</tbody>
</table>

For (0,0,0)' + set

<table>
<thead>
<tr>
<th>(1) 1'</th>
<th>(2) (3^+ \ 0,0,z)</th>
<th>(3) (3^- \ 0,0,z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1'</td>
<td>0,0,0')</td>
<td>(3z'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) 2'</th>
<th>(5) 2' (x,0,0)</th>
<th>(6) 2' (0,y,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2(y)'</td>
<td>0,0,0')</td>
<td>(2(z)'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) (\bar{T}')</th>
<th>(8) (3^+ \ 0,0,z; 0,0,0)</th>
<th>(9) (3^- \ 0,0,z; 0,0,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\bar{T}')</td>
<td>0,0,0')</td>
<td>(3z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) m' (x,\bar{x},z)</th>
<th>(11) m' (x,2x,z)</th>
<th>(12) m' (2x,x,z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m(x)'</td>
<td>0,0,0')</td>
<td>(m(x)'</td>
</tr>
</tbody>
</table>

166.2.1328 - 3 - 2871
Generators selected

\(1\); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(2/3,1/3,1/3)\); \(2\); \(4\); \(7\); \(1\).
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Special Projection</th>
<th>Equation ( * )</th>
<th>Equation ( \ast )</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along ([0,0,1])</td>
<td>(p6mm1')</td>
<td>(a^* = (2a + b)/3)</td>
<td>(b^* = (-a + b)/3)</td>
<td>at 0,0,z</td>
</tr>
<tr>
<td>Along ([1,0,0])</td>
<td>(p2111')</td>
<td>(a^* = (-a - 2b + c)/3)</td>
<td>(b^* = (a + 2b)/2)</td>
<td>at x,0,0</td>
</tr>
<tr>
<td>Along ([2,1,0])</td>
<td>(p2mm1')</td>
<td>(a^* = c/3)</td>
<td>(b^* = b/2)</td>
<td>at x/2,0</td>
</tr>
</tbody>
</table>

Continued

| 18 | \(f\) | \(0.21'\) | \(x,0,0 [0,0,0]\) | \(0,x,0 [0,0,0]\) | \(x,x,0 [0,0,0]\) |
| 9 | \(e\) | \(0.2/m1'\) | \(1/2,0,0 [0,0,0]\) | \(0,1/2,0 [0,0,0]\) | \(1/2,1/2,0 [0,0,0]\) |
| 9 | \(d\) | \(0.2/m1'\) | \(1/2,0,1/2 [0,0,0]\) | \(0,1/2,1/2 [0,0,0]\) | \(1/2,1/2,1/2 [0,0,0]\) |
| 6 | \(c\) | \(3m1'\) | \(0,0,z [0,0,0]\) | \(0,0,z [0,0,0]\) | \(0,0,z [0,0,0]\) |
| 3 | \(b\) | \(\bar{3}m1'\) | \(0,0,1/2 [0,0,0]\) | \(0,0,1/2 [0,0,0]\) | \(0,0,1/2 [0,0,0]\) |
| 3 | \(a\) | \(\bar{3}m1'\) | \(0,0,0 [0,0,0]\) | \(0,0,0 [0,0,0]\) | \(0,0,0 [0,0,0]\) |
R3'\text{m} \\
166.3.1329 \\
\bar{3}'\text{m} \\
R3'2'/m \\

Trigonal
Origin on center ($\overline{3}m$)

**Asymmetric unit**: $0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq y/2; \quad y \leq \min(1-x,2x)$

**Vertices**
- $0,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,0,1/6$
- $2/3,1/3,1/6$
- $1/3,2/3,1/6$
Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 3' 0,0,0
(3) 3' 0,0,0

(4) 2' x,x,0
(2,0,0)'

(5) 2' x,0,0
(2,0,0)'

(6) 2' 0,y,0
(2,0,0)'

(7) 3' 0,0,0; 0,0,0
(3,0,0)'

(9) 3' 0,0,0; 0,0,0
(3,0,0)'

(10) m x,x,z
(m,0,0)

(11) m x,2x,z
(m,0,0)

(12) m 2x,x,z
(m,0,0)

For (2/3,1/3,1/3) + set

(1) t
(1) 2/3,1/3,1/3

(2) 3' 0,0,1/3 1/3,1/3,1/3
(3) 3' 0,0,1/3 1/3,1/3,1/3

(4) 2' (1/2,1/2,0) x,x-1/6,1/6
(2,0,0)'

(5) 2' (1/2,0,0) x,1,1/6
(2,0,0)'

(6) 2' 1/3,y,1/6
(2,0,0)'

(7) 3' 1/3,1/3,1/3; 1/3,1/3,1/3
(3,0,0)'

(8) 3' 1/3,1/3,1/3; 1/3,1/3,1/3
(3,0,0)'

(9) 3' 1/3,2/3,1/3; 1/3,2/3,1/3
(3,0,0)'

(10) g
(1) 1/6,1/6,1/6

(11) g
(1) 1/6,1/6,1/6

(12) g
(1) 1/6,1/6,1/6

For (1/3,2/3,2/3) + set

(1) t
(1) 1/3,2/3,2/3

(2) 3' 0,0,2/3 1/3,2/3,2/3
(3) 3' 0,0,2/3 1/3,2/3,2/3

(4) 2' (1/2,1/2,0) x,x-1/6,1/6
(2,0,0)'

(5) 2' x,1,1/3
(2,0,0)'

(6) 2' 0,1/2,0 1/6,y,1/3
(2,0,0)'

(7) 3' -1/3,1/3,1/3; -1/3,1/3,1/3
(3,0,0)'

(8) 3' -1/3,1/3,1/3; -1/3,1/3,1/3
(3,0,0)'

(9) 3' -1/3,2/3,1/3; -1/3,2/3,1/3
(3,0,0)'

(10) g
(1) -1/6,1/6,2/3

(11) g
(1) -1/6,1/6,2/3

(12) g
(1) -1/6,1/6,2/3

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(2/3,1/3,1/3) +</td>
</tr>
</tbody>
</table>
Continued

36  i  1  (1) x,y,z [u,v,w]  (2) y,x-y,z [v,u-v,w]  (3) x+y,x,z [u+v,u,w]
(4) y,x,z [v,u,w]  (5) x-y,y,z [u+v,v,w]  (6) x,x+y,z [u,u-v,w]
(7) x,y,z [u,v,w]  (8) y,x+y,z [v,u+v,w]  (9) x-y,x,z [u-v,u,w]
(10) y,x,z [v,u,w]  (11) x+y,y,z [u-v,u,w]  (12) x,x-y,z [u,u+v,w]

18 h .m  x,x,z [u,u,0]  x,2x,z [u,0,0]  2x,x,z [0,u,0]
     x,x,z [u,u,0]  2x,x,z [0,u,0]  x,2x,z [u,0,0]
18 g .2'  x,0,1/2 [u,2u,w]  0,x,1/2 [2u,u,w]  x,x,1/2 [u,u,w]
       x,0,1/2 [u,2u,w]  0,x,1/2 [2u,u,w]  x,x,1/2 [u,u,w]
18 f .2'  x,0,0 [u,2u,w]  0,x,0 [2u,u,w]  x,x,0 [u,u,w]
       x,0,0 [u,2u,w]  0,x,0 [2u,u,w]  x,x,0 [u,u,w]

9  e .2/m  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]
9  d .2/m  1/2,0,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]
6  c  3m.  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]
3  b  3'm  0,0,1/2 [0,0,0]  0,0,1/2 [0,0,0]  0,0,1/2 [0,0,0]
3  a  3'm  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p6mm  Along [1,0,0]  p2'11  Along [2,1,0]  p2m'm'
  a* = (2a + b)/3  b* = (-a + b)/3  a* = (-a - 2b + c)/3  b* = (a + 2b)/2
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0

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Origin on center ($\overline{3}m'$)

Asymmetric unit: $0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq y/2; \quad y \leq \min(1-x,2x)$

Vertices:

- $0,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,0,1/6$
- $2/3,1/3,1/6$
- $1/3,2/3,1/6$
Symmetry Operations

For (0,0,0) + set

(1) $1 \quad (1 \parallel 0,0,0)$
(2) $3^+ \quad 0,0,z$  
(3) $3^- \quad 0,0,z$

For (2/3,1/3,1/3) + set

(1) $t \ (2/3,1/3,1/3)$
(2) $3^+ \ (0,0,1/3) \ 1/3,1/3,z$  
(3) $3^- \ (0,0,1/3) \ 1/3,0,z$

For (1/3,2/3,2/3) + set

(1) $t \ (1/3,2/3,2/3)$
(2) $3^+ \ (0,0,2/3) \ 0,1/3,z$  
(3) $3^- \ (0,0,2/3) \ 1/3,1/3,z$

Generators selected  
(1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(2/3,1/3,1/3)$; (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +
### Symmetry of Special Projections

**Along [0,0,1] p6m’m’**
- \(a^* = (2a + b)/3\)
- \(b^* = (-a + b)/3\)
- Origin at 0,0,z

**Along [1,0,0] p211**
- \(a^* = (-a - 2b + c)/3\)
- \(b^* = (a + 2b)/2\)
- Origin at x,0,0

**Along [2,1,0] p2m’m’**
- \(a^* = c/3\)
- \(b^* = b/2\)
- Origin at x,x/2,0

---

Continued

166.4.1330

R3’m’

36  i  1  (1) x,y,z [u,v,w]  
     (4) y,x,z [v,u,w]  
     (7) x,y,z [u,v,w]  
     (10) y,x,z [v,u,w]  

18  h .m’  x,x,z [u,u,w]  
     x,2x,z [u,2u,w]  
18  g .2  x,0,1/2 [u,0,0]  
     0,x,1/2 [0,u,0]  
18  f .2  x,0,0 [u,0,0]  
     0,x,0 [0,u,0]  
9   e .2/m’  1/2,0,0 [0,0,0]  
     0,1/2,0 [0,0,0]  
9   d .2/m’  1/2,0,1/2 [0,0,0]  
     0,1/2,1/2 [0,0,0]  
6   c  3m’  0,0,z [0,0,w]  
     0,0,z [0,0,w]  
3   b  3’m’  0,0,1/2 [0,0,0]  
3   a  3’m’  0,0,0 [0,0,0]  

---

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Origin on center ($\overline{3}m'$)

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 < z < 1/6; \quad x < y/2; \quad y < \min(1-x, 2x) \]

Vertices

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices</td>
<td>0,0,0</td>
<td>2/3,1/3,0</td>
<td>1/3,2/3,0</td>
</tr>
<tr>
<td></td>
<td>0,0,1/6</td>
<td>2/3,1/3,1/6</td>
<td>1/3,2/3,1/6</td>
</tr>
</tbody>
</table>
### Symmetry Operations

**For (0,0,0) + set**

1. \((1)\) 1
2. \((2)\) 3\(^*\) 0,0,z
3. \((3)\) 3\(^*\) 0,0,z
4. \((4)\) 2\' x,x,0
5. \((5)\) 2\' x,0,0
6. \((6)\) 2\' 0,y,0
7. \((7)\) \(\bar{1}\)
8. \((8)\) 3\(^*\) 0,0,z; 0,0,0
9. \((9)\) 3\(^*\) 0,0,z; 0,0,0
10. \((10)\) m\' x,x,z
11. \((11)\) m\' x,2x,z
12. \((12)\) m\' 2x,x,z

**For \((2/3,1/3,1/3) + set**

1. \((1)\) t \((2/3,1/3,1/3)
2. \((2)\) 3\(^*\) (0,0,1/3) 1/3,1/3,z
3. \((3)\) 3\(^*\) (0,0,1/3) 1/3,0,z
4. \((4)\) 2\' (1/2,1/2,0) x,x-1/6,1/6
5. \((5)\) 2\' (1/2,0,0) x,1/6,1/6
6. \((6)\) 2\' 1/3,y,1/6
7. \((7)\) \(\bar{1}\)
8. \((8)\) 3\(^*\) 1/3,-1/3,z; 1/3,-1/3,1/3
9. \((9)\) 3\(^*\) 1/3,2/3,z; 1/3,2/3,1/6
10. \((10)\) g\' (1/6,-1/6,1/3)
11. \((11)\) g\' (1/6,1/3,1/3)
12. \((12)\) g\' (2/3,1/3,1/3)

**For \((1/3,2/3,2/3) + set**

1. \((1)\) t \((1/3,2/3,2/3)
2. \((2)\) 3\(^*\) (0,0,2/3) 0,1/3,z
3. \((3)\) 3\(^*\) (0,0,2/3) 1/3,1/3,z
4. \((4)\) 2\' (1/2,1/2,0) x,x+1/6,1/3
5. \((5)\) 2\' x,1/3,1/3
6. \((6)\) 2\' (0,1/2,0) 1/6,y,1/3
7. \((7)\) \(\bar{1}\)
8. \((8)\) 3\(^*\) 2/3,1/3,1/3
9. \((9)\) 3\(^*\) -1/3,1/3,z; -1/3,1/3,1/3
10. \((10)\) g\' (-1/6,1/6,2/3)
11. \((11)\) g\' (1/3,2/3,2/3)
12. \((12)\) g\' (1/3,1/6,2/3)

**Generators selected**: \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).**

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
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<tbody>
<tr>
<td>((0,0,0)) + ((2/3,1/3,1/3)) + ((1/3,2/3,2/3))</td>
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</table>
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Symmetry</th>
<th>Origin</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>p2'11</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>p2mm'</td>
<td>[x,x/2,0]</td>
</tr>
<tr>
<td>3</td>
<td>p6'1m</td>
<td>[0,0,z]</td>
</tr>
</tbody>
</table>

### p6'1m

- Origin at 0,0,z
- \( a^* = \frac{2a + b}{3} \)
- \( b^* = \frac{-a + b}{3} \)

### p2mm'

- Origin at x,x/2,0
- \( a^* = c/3 \)
- \( b^* = b/2 \)

### p2'11

- \( a^* = \frac{-a - 2b + c}{3} \)
- \( b^* = \frac{a + 2b}{2} \)
Origin on center (3m)

Asymmetric unit: 
\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/6; \quad x \leq y/2; \quad y \leq \min(1-x, 2x) \]

Vertices:
- \( 0,0,0 \)
- \( 2/3,1/3,0 \)
- \( 1/3,2/3,0 \)
- \( 0,0,1/6 \)
- \( 2/3,1/3,1/6 \)
- \( 1/3,2/3,1/6 \)
### Symmetry Operations

For \((0,0,0) + \) set

1. \((1) \ 1 \ (1 \ 0,0,0)\)
2. \((2) \ 3^* \ 0,0,z \ (3) \ 3^* \ 0,0,z \ (3z) \ 0,0,0 \ (3z^*) \ 0,0,0\)
3. \((2) \ x,x,0 \ (2) \ 0,0,0 \ (6) \ 0,0,0 \ (2y) \ 0,0,0\)
4. \((7) \ T \ (1 \ 0,0,0) \ (8) \ 3^* \ 0,0,z; 0,0,0 \ (9) \ 3^* \ 0,0,z; 0,0,0 \ (3z) \ 0,0,0 \ (3z^*) \ 0,0,0\)
5. \((10) \ m \ x,x,z \ (m_{\alpha}) \ 0,0,0 \ (12) \ m \ 2x,x,z \ (m_{\gamma}) \ 0,0,0\)

For \((2/3,1/3,1/3) + \) set

1. \((1) \ t' \ (2/3,1/3,1/3) \ (2) \ 3^* \ (0,0,1/3) \ (3) \ 3^* \ (0,0,1/3) \ (3z) \ 2/3,1/3,1/3 \ (3z^*) \ 2/3,1/3,1/3\)
2. \((4) \ 2' \ (1/2,0,0) \ x,1/6,1/6 \ (5) \ 2' \ (1/2,1/2,0) \ x,x-1/6,1/6 \ (2x) \ 2/3,1/3,1/3 \ (2y) \ 2/3,1/3,1/3 \ (2z) \ 2/3,1/3,1/3\)
3. \((7) \ T \ (1 \ 3/2,1/3,1/3) \ (8) \ 3^* \ 1/3,-1/3,z; 1/3,-1/3,1/6 \ (9) \ 3^* \ 1/3,2/3,z; 1/3,2/3,1/6 \ (3z) \ 2/3,1/3,1/3 \ (3z^*) \ 2/3,1/3,1/3\)
4. \((10) \ g' \ (1/6,-1/6,1/3) \ x+1/2,x,z \ (11) \ g' \ (1/6,1/3,1/3) \ x,2x-1/2,z \ (12) \ g' \ (2/3,1/3,1/3) \ 2x,x,z \ (m_{\alpha}) \ 2/3,1/3,1/3 \ (m_{\beta}) \ 2/3,1/3,1/3 \ (m_{\gamma}) \ 2/3,1/3,1/3\)

For \((1/3,2/3,2/3) + \) set

1. \((1) \ t \ (1/3,2/3,2/3) \ (2) \ 3^* \ (0,0,2/3) \ 0,1/3,z \ (3) \ 3^* \ (0,0,2/3) \ 1/3,1/3,z \ (3z) \ 1/3,2/3,2/3 \ (3z^*) \ 1/3,2/3,2/3\)
2. \((4) \ 2 \ (1/2,1/2,0) \ x,x+1/6,1/3 \ (5) \ 2 \ x,1/3,1/3 \ (6) \ 2 \ (0,1/2,0) \ 1/6,y,1/3 \ (2x) \ 1/3,2/3,2/3 \ (2y) \ 1/3,2/3,2/3 \ (2z) \ 1/3,2/3,2/3\)
3. \((7) \ T \ (1 \ 1/3,2/3,2/3) \ (8) \ 3^* \ 2/3,1/3,z; 2/3,1/3,1/3 \ (9) \ 3^* \ -1/3,1/3,z; -1/3,1/3,1/3 \ (3z) \ 1/3,2/3,2/3 \ (3z^*) \ 1/3,2/3,2/3\)
4. \((10) \ g \ (-1/6,1/6,2/3) \ x+1/2,x,z \ (11) \ g \ (1/3,2/3,2/3) \ x,2x,z \ (12) \ g \ (1/3,1/3,2/3) \ 2x-1/2,x,z \ (m_{\alpha}) \ 1/3,2/3,2/3 \ (m_{\beta}) \ 1/3,2/3,2/3 \ (m_{\gamma}) \ 1/3,2/3,2/3\)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(2/3,1/3,1/3); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(2/3,1/3,1/3) +</td>
<td>(1/3,2/3,2/3) +</td>
</tr>
<tr>
<td>36</td>
<td>i</td>
<td>1</td>
</tr>
<tr>
<td>36</td>
<td>i</td>
<td>1</td>
</tr>
<tr>
<td>36</td>
<td>i</td>
<td>1</td>
</tr>
<tr>
<td>36</td>
<td>i</td>
<td>1</td>
</tr>
</tbody>
</table>

18 | h | m | x, x, z [u, u, 0] | x, 2x, z [u, 0, 0] | 2x, x, z [0, u, 0] |
| 18 | h | m | x, x, z [u, u, 0] | 2x, x, z [0, u, 0] | x, 2x, z [u, 0, 0] |

18 | g | .2' | x, 0, 1/2 [u, 2u, w] | 0, x, 1/2 [2u, u, w] | x, x, 1/2 [u, u, w] |
| 18 | g | .2' | x, 0, 1/2 [u, 2u, w] | 0, x, 1/2 [2u, u, w] | x, x, 1/2 [u, u, w] |

18 | f | .2 | x, 0, 0 [u, 0, 0] | 0, x, 0 [0, u, 0] | x, x, 0 [u, u, 0] |
| 18 | f | .2 | x, 0, 0 [u, 0, 0] | 0, x, 0 [0, u, 0] | x, x, 0 [u, u, 0] |

9 | e | .2/m | 1/2, 0, 0 [u, 0, 0] | 0, 1/2, 0 [0, u, 0] | 1/2, 1/2, 0 [u, u, 0] |
| 9 | e | .2/m | 1/2, 0, 1/2 [0, 0, 0] | 0, 1/2, 1/2 [0, 0, 0] | 1/2, 1/2, 1/2 [0, 0, 0] |

6 | c | 3m | 0, 0, z [0, 0, 0] | 0, 0, z [0, 0, 0] |

3 | b | 3m | 0, 0, 1/2 [0, 0, 0] |

3 | a | 3m | 0, 0, 0 [0, 0, 0] |

**Symmetry of Special Projections**

Along [0, 0, 1] p6mm1'  
\[ \mathbf{a}^* = \frac{2a+b}{3}, \quad \mathbf{b}^* = \frac{-a+b}{3} \]  
Origin at 0, 0, z

Along [1, 0, 0] p2111'  
\[ \mathbf{a}^* = \frac{-a-2b+c}{3}, \quad \mathbf{b}^* = \frac{a+2b}{2} \]  
Origin at x, 0, 0

Along [2, 1, 0] p2a, 2mm  
\[ \mathbf{a}^* = \frac{c}{3}, \quad \mathbf{b}^* = b/2 \]  
Origin at x, x/2, 1/6
Origin on center (3m')

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{6}; \quad x \leq \frac{y}{2}; \quad y \leq \min(1-x,2x) \]

Vertices

- \( 0,0,0 \)
- \( 2/3,1/3,0 \)
- \( 1/3,2/3,0 \)
- \( 0,0,1/6 \)
- \( 2/3,1/3,1/6 \)
- \( 1/3,2/3,1/6 \)
### Symmetry Operations

For \((0,0,0) + \) set

| (1) \(1 \) | (2) \( 3^+ \) \(0,0,z\) | (3) \( 3^- \) \(0,0,z\) |
| \((1,0,0)\) | \((3_z,0,0,0)\) | \((3_z^{-1},0,0,0)\) |
| (4) \(2' \) \(x,x,0\) | (5) \( 2' \) \(x,0,0\) | (6) \( 2' \) \(0,y,0\) |
| \((2\sqrt{y}|0,0,0)\)' | \((2\sqrt{z}|0,0,0)\)' | \((2\sqrt{y}|0,0,0)\)' |
| (7) \(\bar{T} \) | (8) \( 3^+ \) \(0,0,z;0,0,0\) | (9) \( 3^- \) \(0,0,z;0,0,0\) |
| \((\bar{T}|0,0,0)\) | \((3_z|0,0,0)\) | \((3_z^{-1}|0,0,0)\) |
| (10) \(m' \) \(x,x,z\) | (11) \(m' \) \(x,2x,z\) | (12) \(m' \) \(2x,x,z\) |
| \((m_{xy}|0,0,0)'\) | \((m_{xy}|0,0,0)'\) | \((m_{xy}|0,0,0)'\) |

For \((2/3,1/3,1/3)' + \) set

| (1) \(t\) \((2/3,1,3/3)\) | (2) \( 3^+ \) \((0,0,1/3)\) \(1/3,1/3,z\) |
| \((1,2/3,1/3,1/3)'\) | \((3_z|2/3,1,3/3,1/3)'\) | \((3_z^{-1}|2/3,1,3/3,1/3)'\) |
| (4) \(2\) \((2/3,1/3,1/3)\) \(x,-x,1/6,1/6\) | (5) \( 2\) \((1/2,0,0)\) \(x,1/6,1/6\) |
| \((2\sqrt{y}|2/3,1,3/3,1/3)'\) | \((2\sqrt{z}|2/3,1,3/3,1/3)'\) | \((2\sqrt{y}|2/3,1,3/3,1/3)'\) |
| (7) \(\bar{T} \) \(1/3,1,6,1/6\) | (8) \( 3^+ \) \((1/3,-1/3,z;1/3,-1/3,1/6)\) |
| \((\bar{T}|2/3,1,3,1/3)'\) | \((3_z|2/3,1,3,1/3)'\) | \((3_z^{-1}|2/3,1,3,1/3)'\) |
| (10) \(g\) \((1/6,-1/6,1/3)\) \(x+1/2,x,z\) | (11) \(g\) \((1/6,1/3,1/3)\) \(x,2x-1/2,z\) |
| \((m_{xy}|2/3,1,3,1/3)'\) | \((m_{xy}|2/3,1,3,1/3)'\) | \((m_{xy}|2/3,1,3,1/3)'\) |

For \((1/3,2/3,2/3) + \) set

| (1) \(t\) \((1/3,2,3/3)\) | (2) \( 3^+ \) \((0,0,2/3)\) \(0,1/3,z\) |
| \((1,1/3,2,3/3)'\) | \((3_z|1/3,2,3,2/3)'\) | \((3_z^{-1}|1/3,2,3,2/3)'\) |
| (4) \(2'\) \((1/2,1/2,0)\) \(x,x+1/6,1/3\) | (5) \( 2'\) \((1/2,1/2,0)\) \(x,1/3,1/3\) |
| \((2\sqrt{y}|1/3,2,3,2/3)'\) | \((2\sqrt{z}|1/3,2,3,2/3)'\) | \((2\sqrt{y}|1/3,2,3,2/3)'\) |
| (7) \(\bar{T} \) \(1/3,1,6,1/3\) | (8) \( 3^+ \) \((2/3,1,3,1/3)\) \(2/3,1,3,1/3\) |
| \((\bar{T}|1/3,2,3,2/3)'\) | \((3_z|2/3,1,3,1/3)'\) | \((3_z^{-1}|2/3,1,3,1/3)'\) |
| (10) \(g'\) \((-1/6,1/6,1/3)\) \(x+1/2,x,z\) | (11) \(g'\) \((1/3,2,3,2/3)\) \(x,2x,z\) |
| \((m_{xy}|1/3,2,3,2/3)'\) | \((m_{xy}|1/3,2,3,2/3)'\) | \((m_{xy}|1/3,2,3,2/3)'\) |

Generators selected  
\(1)\); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t'(2/3,1,3/1,3)\); \(2)\); \(4)\); \(7)\).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0)) + ((2/3,1,3,1/3)') + ((1/3,2,3,2/3))</td>
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</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p6mm1'</td>
<td>0,0,z</td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p2a 211</td>
<td>0,0,0</td>
</tr>
<tr>
<td>[2,1,0]</td>
<td>p2a* 2m'm'</td>
<td>x,x/2,1/6</td>
</tr>
</tbody>
</table>

**a*** = (2a + b)/3  
**b*** = (-a + b)/3

Origin at 0,0,z

**a*** = (-a - 2b + c)/3  
**b*** = (a + 2b)/2

Origin at x-1/6,-1/3,1/6

**a*** = b/2  
**b*** = c/3

Origin at x,x/2,1/6

---

**Continued**

<table>
<thead>
<tr>
<th>36</th>
<th>i</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) y,x-y,z [v,u-v,w]</th>
<th>(3) x+y,x,z [u+v,u,w]</th>
</tr>
</thead>
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<tr>
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<td>(4) y,x,z [v,u,w]</td>
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<td>(5) x-y,x,z [u+v,w]</td>
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<td>(6) x,x+y,z [u,v,w]</td>
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<td>(7) x,y,z [u,v,w]</td>
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<td>(8) y,x+y,z [v,u-w]</td>
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<td>(9) x-y,x,z [u-v,u,w]</td>
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<td>(10) y,x,z [v,u,w]</td>
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<td>(11) x+y,y,z [u+v,v,w]</td>
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<td>(12) x,x-y,z [u,u-v,w]</td>
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</tbody>
</table>

18 h .m' x,x,z [u,u,w]  
2x,x,z [2u,u,w]

18 g .2 x,0,1/2 [u,0,0]  
0,x,1/2 [0,u,0]

18 f .2' x,0,0 [u,2u,w]  
0,x,0 [2u,u,w]

9 e .2'/m' 1/2,0,0 [u,2u,w]  
0,1/2,0 [2u,u,w]  
1/2,1/2,0 [u,u,w]

9 d .2/m' 1/2,0,1/2 [0,0,0]  
0,1/2,1/2 [0,0,0]  
1/2,1/2,1/2 [0,0,0]

6 c 3m' 0,0,z [0,0,0]  
0,0,z [0,0,w]

3 b 3m' 0,0,1/2 [0,0,w]

3 a 3m' 0,0,0 [0,0,w]  

---

**166.7.1333**

**R*** = 3m'
Origin on (3) at 3c

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/12; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \]

Vertices

- \(0,0,0\)
- \(0,0,1/12\)
- \(1/2,0,0\)
- \(1/2,0,1/12\)
- \(2/3,1/3,0\)
- \(2/3,1/3,1/12\)
- \(1/3,2/3,0\)
- \(1/3,2/3,1/12\)
- \(0,1/2,0\)
- \(0,1/2,1/12\)
### Symmetry Operations

For (0,0,0) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
</tr>
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<tbody>
<tr>
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<td>$t(0,0,0)$</td>
<td>(0,0,0)</td>
<td>1; t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); t(2,1/2,0)</td>
</tr>
<tr>
<td>2</td>
<td>$x,x,1/4$</td>
<td>(2x,0,0,1/2)</td>
<td>2; 2x,0,1/4; 2x,0,1/2</td>
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<tr>
<td>3</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>3; 0,0,0; 3z,0,0,0</td>
</tr>
<tr>
<td>4</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>4; 2x,0,1/4; 2x,0,1/2</td>
</tr>
<tr>
<td>5</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>5; 0,0,0; 5z,0,0,0</td>
</tr>
<tr>
<td>6</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>6; 0,y,1/4; 0,y,1/2</td>
</tr>
<tr>
<td>7</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>7; 0,0,0; 7z,0,0,0</td>
</tr>
<tr>
<td>8</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>8; 2x,0,1/4; 2x,0,1/2</td>
</tr>
<tr>
<td>9</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>9; 0,0,0; 9z,0,0,0</td>
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</tbody>
</table>

For (2/3,1/3,1/3) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$t(2/3,1/3,1/3)$</td>
<td>(2x,0,0,1/2)</td>
<td>1; t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); t(2,1/2,0)</td>
</tr>
<tr>
<td>2</td>
<td>$x,x-1,6,5/12$</td>
<td>(2x,0,0,1/2)</td>
<td>2; x,1,6,5/12; 2x,1,6,5/12</td>
</tr>
<tr>
<td>3</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>3; 0,0,0; 3z,0,0,0</td>
</tr>
<tr>
<td>4</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>4; 2x,1,6,5/12; 2x,1,6,5/12</td>
</tr>
<tr>
<td>5</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>5; 0,0,0; 5z,0,0,0</td>
</tr>
<tr>
<td>6</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>6; 0,y,1,6,5/12; 0,y,1,6,5/12</td>
</tr>
<tr>
<td>7</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>7; 0,0,0; 7z,0,0,0</td>
</tr>
<tr>
<td>8</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>8; 2x,1,6,5/12; 2x,1,6,5/12</td>
</tr>
<tr>
<td>9</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>9; 0,0,0; 9z,0,0,0</td>
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For (1/3,2,3/2,3) + set

<table>
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<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
</tr>
</thead>
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<tr>
<td>1</td>
<td>$t(1/3,2,3/2,3)$</td>
<td>(2x,0,0,1/2)</td>
<td>1; t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); t(2,1/2,0)</td>
</tr>
<tr>
<td>2</td>
<td>$x,x+1,6,1/12$</td>
<td>(2x,0,0,1/2)</td>
<td>2; x,1,6,1/12; 2x,1,6,1/12</td>
</tr>
<tr>
<td>3</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>3; 0,0,0; 3z,0,0,0</td>
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<tr>
<td>4</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>4; 2x,1,6,1/12; 2x,1,6,1/12</td>
</tr>
<tr>
<td>5</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>5; 0,0,0; 5z,0,0,0</td>
</tr>
<tr>
<td>6</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>6; 0,y,1,6,1/12; 0,y,1,6,1/12</td>
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<tr>
<td>7</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>7; 0,0,0; 7z,0,0,0</td>
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<tr>
<td>8</td>
<td>$2$</td>
<td>(2x,0,0,1/2)</td>
<td>8; 2x,1,6,1/12; 2x,1,6,1/12</td>
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<tr>
<td>9</td>
<td>$1$</td>
<td>(0,0,0)</td>
<td>9; 0,0,0; 9z,0,0,0</td>
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</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); t(2,1/2,0); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
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<tbody>
<tr>
<td>(0,0,0) + (2/3,1/3,1/3) + (1/3,2,3/2,3) +</td>
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<td>36</td>
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<tr>
<td>6</td>
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<tr>
<td>6</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6\textsuperscript{mm'}
\( \mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3 \)
\( \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/3 \)
Origin at 0,0,z

Along [1,0,0] \( p_{2\text{mm}}^\prime 211 \)
\( \mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6 \)
\( \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)
Origin at x,0,1/4

Along [2,1,0] p2\textsuperscript{m'g}
\( \mathbf{a}^* = \mathbf{c}/3 \)
\( \mathbf{b}^* = \mathbf{b}/2 \)
Origin at x,x/2,0
Origin on \((3'1')\) at \(\bar{3}c1'\)

Asymmetric unit

\[0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/12; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)\]

Vertices

\[
\begin{array}{cccc}
0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/3,2/3,0 \\
0,0,1/12 & 1/2,0,1/12 & 2/3,1/3,1/12 & 1/3,2/3,1/12 \\
& & & 0,1/2,0 \\
& & & 0,1/2,1/12
\end{array}
\]
Symmetry Operations

For (0,0,0) + set

(1) 1
(1') 0,0,0)
(2) 3' 0,0,0 (3' 0,0,0 (3' 0,0,0)
(3) 3' 0,0,0 (3' 0,0,0 (3' 0,0,0)
(4) 2 x.x,1/4
(2y) 0,0,1/2)
(5) 2 x,0,1/4 (6) 2 0,y,1/4 (6) 2 0,y,1/4
(2y) 0,0,1/2)
(7) T
(T' 0,0,0)
(8) 3' 0,0,0; 0,0,0 (9) 3' 0,0,0; 0,0,0
(3' 0,0,0) (3' 0,0,0)
(10) c (0,0,1/2) x,x,z (11) c (0,0,1/2) x,2x,z (12) c (0,0,1/2) 2x,x,z
(my) 0,0,1/2)
(my) 0,0,1/2)
(my) 0,0,1/2)

For (2/3,1/3,1/3) + set

(1) t (2/3,1/3,1/3)
(1) 2/3,1/3,1/3)
(2) 3' (0,0,1/3) 1/3,1/3,z (3) 3' (0,0,1/3) 1/3,0,z
(3') 2/3,1/3,1/3)
(3') 2/3,1/3,1/3)
(4) 2(1/2,1/2,0) x,x-1,6,5/12
(2y) 2/3,1/3,5/6)
(5) 2 (1/2,0,0) x,1,6,5/12 (6) 2 1/3,y,5/12
(2y) 2/3,1/3,5/6)
(2y) 2/3,1/3,5/6)
(7) T
(T' 1/3,1/3,1/3)
(8) 3' 1/3,1/3,1/3; 1/3,-1/3,1/3 (9) 3' 1/3,2,3/3; 1/3,2,3/3
(3' 1/3,1/3,1/3) (3' 1/3,2,3/3)
(3' 1/3,1/3,1/3) (3' 1/3,2,3/3)
(10) g (1/6,-1/6,5/6) x+1/2,x,z (11) g (1/6,1/3,5/6) x,2x-1/2,z (12) g (2/3,1/3,5/6) 2x,x,z
(my) 2/3,1/3,5/6)
(my) 2/3,1/3,5/6)
(my) 2/3,1/3,5/6)

For (1/3,2,3/2) + set

(1) t (1/3,2,3/2)
(1') 1/3,2,3/2)
(2) 3' (0,0,2/3) 0,1/3,z (3) 3' (0,0,2/3) 1/3,1/3,z
(3') 1/3,2,3/2)
(3') 1/3,2,3/2)
(4) 2(1/2,1/2,0) x,x-1,6,5/12
(2y) 1/3,2,3/1/6)
(5) 2 (1/2,1/2,0) x,1,6,5/12 (6) 2 0,1/2,0 1/6,y,1/2
(2y) 1/3,2,3/1/6)
(2y) 1/3,2,3/1/6)
(7) T
(T' 1/3,2,3/2,3)
(8) 3' 2/3,1/3,3; 2/3,1/3,3 (9) 3' -1/3,1/3,3; -1/3,1/3,3
(3' 2/3,1/3,3) (3' 1/3,2,3/2,3)
(3' 2/3,1/3,3) (3' 1/3,2,3/2,3)
(10) g (-1/6,1/6,1/6) x+1/2,x,z (11) g (1/6,1/3,5/6) x,2x-1/2,z (12) g (2/3,1/3,5/6) 2x,x,z
(my) 1/3,2,3/1/6)
(my) 1/3,2,3/1/6)
(my) 1/3,2,3/1/6)

For (0,0,0)' + set

(1) 1'
(1' 0,0,0)'
(2) 3' 0,0,0 (3' 0,0,0 (3' 0,0,0)
(3) 3' 0,0,0 (3' 0,0,0 (3' 0,0,0)
(4) 2' x,x,1/4
(2y) 0,0,1/2)
(5) 2' x,0,1/4 (6) 2' 0,y,1/4 (6) 2' 0,y,1/4
(2y) 0,0,1/2)
(2y) 0,0,1/2)
(7) T'
(T' 0,0,0)'
(8) 3' 0,0,0; 0,0,0 (9) 3' 0,0,0; 0,0,0
(3' 0,0,0) (3' 0,0,0)
(3' 0,0,0) (3' 0,0,0)
(10) c' (0,0,1/2) x,x,z (11) c' (0,0,1/2) x,2x,z (12) c' (0,0,1/2) 2x,x,z
(my) 0,0,1/2)
(my) 0,0,1/2)
(my) 0,0,1/2)
For \( (2/3,1/3,1/3)' + \text{set} \)

**Generators selected**

\( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7); 1' \).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( (0,0,0) + )</td>
<td>( (0,0,0)' + )</td>
</tr>
<tr>
<td>36 f 11'</td>
<td>(1) ( x,y,z [0,0,0] )</td>
</tr>
<tr>
<td>18 e .21'</td>
<td>(7) ( x,y,z [0,0,0] )</td>
</tr>
<tr>
<td>18 d 11'</td>
<td>(13) ( x,y,z+1/2 [0,0,0] )</td>
</tr>
<tr>
<td>12 c 3.1'</td>
<td>(19) ( y,x,x+1/2 [0,0,0] )</td>
</tr>
</tbody>
</table>
Continued

6 b \(\overline{3}.1'\) 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]
6 a 321' 0,0,1/4 [0,0,0] 0,0,3/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p6mm1'
\(a^* = (2a + b)/3\) \(b^* = (-a + b)/3\)
Origin at 0,0,z

Along [1,0,0] p 2111'
\(a^* = (2a + 4b + c)/6\) \(b^* = (a + 2b)/2\)
Origin at x,0,0

Along [2,1,0] p2mg1'
\(a^* = c/3\) \(b^* = b/2\)
Origin at x,x/2,0
Origin on (3') at 3c

Asymmetric unit

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; 0 ≤ z ≤ 1/12; x ≤ (1+y)/2; y ≤ min(1-x,(1+x)/2)

Vertices

0,0,0 1/2,0,0 2/3,1/3,0 1/3,2/3,0 0,1/2,0
0,0,1/12 1/2,0,1/12 2/3,1/3,1/12 1/3,2/3,1/12 0,1/2,1/12
Symmetry Operations

For (0,0,0) + set

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<th>0,0,z</th>
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</thead>
<tbody>
<tr>
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<td>3'</td>
<td>0,0,z</td>
</tr>
<tr>
<td>(2)</td>
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</tr>
<tr>
<td>(3)</td>
<td>3'</td>
<td>0,0,z</td>
</tr>
<tr>
<td>(3')</td>
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<table>
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<td>(5)</td>
<td>2'</td>
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</tr>
<tr>
<td>(6)</td>
<td>0,y,1/4</td>
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<tr>
<td>(6')</td>
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<table>
<thead>
<tr>
<th>(7)</th>
<th>T°</th>
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</tr>
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<tbody>
<tr>
<td>(8)</td>
<td>3'</td>
<td>0,0,0</td>
</tr>
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<td>(9)</td>
<td>3'</td>
<td>0,0,0</td>
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<table>
<thead>
<tr>
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<th>c</th>
<th>(0,0,1/2) x,x,z</th>
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<tbody>
<tr>
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<td>(0,0,1/2) x,2x,z</td>
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<tr>
<td>(12)</td>
<td>c</td>
<td>(0,0,1/2) 2x,x,z</td>
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For (2/3,1/3,1/3) + set

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<tbody>
<tr>
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<tr>
<td>(3)</td>
<td>3'</td>
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</tr>
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<td>(3')</td>
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<table>
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<tbody>
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<table>
<thead>
<tr>
<th>(7)</th>
<th>T°</th>
<th>1/3,1/6,1/6</th>
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</thead>
<tbody>
<tr>
<td>(8)</td>
<td>3'</td>
<td>1/3,-1/3,z</td>
</tr>
<tr>
<td>(9)</td>
<td>3'</td>
<td>1/3,-1/3,z</td>
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</tbody>
</table>

<table>
<thead>
<tr>
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<th>g</th>
<th>(1/6,1,3,5/6) x+x,z</th>
</tr>
</thead>
<tbody>
<tr>
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<td>g</td>
<td>(1/6,1,3,5/6) x,2x-1/2,z</td>
</tr>
<tr>
<td>(12)</td>
<td>g</td>
<td>(1/6,1,3,5/6) 2x,x,z</td>
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For (1/3,2,3,2/3) + set

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</tr>
</thead>
<tbody>
<tr>
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<tr>
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<td>3'</td>
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<table>
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<td>x,1/6,5/12</td>
</tr>
<tr>
<td>(6)</td>
<td>0,y,5/12</td>
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</tr>
<tr>
<td>(6')</td>
<td>0,0,1/6</td>
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<table>
<thead>
<tr>
<th>(7)</th>
<th>T°</th>
<th>1/3,2,3,2/3</th>
</tr>
</thead>
<tbody>
<tr>
<td>(8)</td>
<td>3'</td>
<td>2/3,1/3,z</td>
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<tr>
<td>(9)</td>
<td>3'</td>
<td>-1/3,1/3,z</td>
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<table>
<thead>
<tr>
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<th>g</th>
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</thead>
<tbody>
<tr>
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<td>(1/3,2,3,1/6) x,x,z</td>
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<tr>
<td>(12)</td>
<td>g</td>
<td>(1/3,2,3,1/6) 2x-1/2,x,z</td>
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</tbody>
</table>

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coordinates</td>
</tr>
</tbody>
</table>

(0,0,0) + (2/3,1/3,1/3) + (1/3,2,3,2/3) +
Continued

36  f  1

(1) \( x,y,z \ [u,v,w] \)

(2) \( y,x-y,z \ [v,v+u+w] \)

(3) \( \bar{x+y,x,z} \ [u+v,u,w] \)

(4) \( y,x,z+\frac{1}{2} \ [v,u,w] \)

(5) \( x-y,x,z+\frac{1}{2} \ [u+v+u,w] \)

(6) \( x,x+y,z+\frac{1}{2} \ [u,u-v,w] \)

(7) \( x,y,z \ [u,v,w] \)

(8) \( y,x+y,z \ [v,u+v,w] \)

(9) \( x-y,x,z \ [u-v,u,w] \)

(10) \( \bar{y},x,z+\frac{1}{2} \ [v,u+w] \)

(11) \( x+y,y,z+\frac{1}{2} \ [u-v,u,w] \)

(12) \( x,x-y,z+\frac{1}{2} \ [u,u+v,w] \)

18  e  .2'

(1) \( x,0,1/4 \ [u,2u,w] \)

(2) \( x,0,1/4 \ [v,2u,u] \)

(3) \( \bar{x},x,1/4 \ [u,u,w] \)

18  d  \( \bar{1}' \)

(1) \( 1/2,0,0 \ [0,0,0] \)

(2) \( 1/2,0,1/2 \ [0,0,0] \)

(3) \( 0,1/2,1/2 \ [0,0,0] \)

12  c  3.

(1) \( 0,0,0 \ [0,0,0] \)

(2) \( 0,0,1/2 \ [0,0,0] \)

6  b  32'

(1) \( 0,0,1/4 \ [0,0,0] \)

(2) \( 0,0,1/4 \ [0,0,0] \)

(3) \( 0,0,3/4 \ [0,0,0] \)

Symmetry of Special Projections

Along \([0,0,1]\) p6mm
\(a^* = (2a + b)/3\)
\(b^* = (-a + b)/3\)
Origin at 0,0,z

Along \([1,0,0]\) p 2111'
\(a^* = (2a + 4b + c)/6\)
\(b^* = (a + 2b)/2\)
Origin at x,0,0

Along \([2,1,0]\) p2mg
\(a^* = c/3\)
\(b^* = b/2\)
Origin at x,x/2,0
Origin on (3') at 3c'

**Asymmetric unit**

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/12; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \]

**Vertices**

- \(0,0,0\)
- \(1/2,0,0\)
- \(2/3,1/3,0\)
- \(1/3,2/3,0\)
- \(0,1/2,0\)
- \(0,0,1/12\)
- \(1/2,0,1/12\)
- \(2/3,1/3,1/12\)
- \(1/3,2/3,1/12\)
- \(0,1/2,1/12\)
### Symmetry Operations

**For (0,0,0) + set**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(0,0,0)</td>
</tr>
<tr>
<td>(1) 0,0,0</td>
<td>(3z,0,0,0)</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>0,0,z</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>0,0,0</td>
</tr>
<tr>
<td>(2) x,x,1/4</td>
<td>x,0,1/4</td>
</tr>
<tr>
<td>(2) 0,0,1/2</td>
<td>0,0,1/2</td>
</tr>
<tr>
<td>(4) 2</td>
<td>0,1/4</td>
</tr>
<tr>
<td>(4) x</td>
<td>0,1/4</td>
</tr>
<tr>
<td>(5) 2</td>
<td>0,0,1/2</td>
</tr>
<tr>
<td>(6) 2</td>
<td>0,0,1/2</td>
</tr>
<tr>
<td>(7) T^+</td>
<td>0,0,z; 0,0,0</td>
</tr>
<tr>
<td>(7) 0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>(7) T^-</td>
<td>0,0,z; 0,0,0</td>
</tr>
<tr>
<td>(7) 0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>(8) c'</td>
<td>(0,0,1/2) x,2x,z</td>
</tr>
<tr>
<td>(9) c'</td>
<td>(0,0,1/2) 2x,x,z</td>
</tr>
</tbody>
</table>

**For (2/3,1/3,1/3) + set**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t</td>
<td>(2/3,1/3,1/3)</td>
</tr>
<tr>
<td>(1) 2/3,1/3,1/3</td>
<td>2/3,1/3,1/3</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>0,0,1/3</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>1/3,1/3,z</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>0,0,1/3</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>1/3,1/3,z</td>
</tr>
<tr>
<td>(4) 2</td>
<td>x,x-1/6,1/12</td>
</tr>
<tr>
<td>(4) 2</td>
<td>x,1/6,5/12</td>
</tr>
<tr>
<td>(5) 2</td>
<td>1/2,1/3,1/2</td>
</tr>
<tr>
<td>(5) 2</td>
<td>1/2,1/3,1/2</td>
</tr>
<tr>
<td>(6) 2</td>
<td>1/3,y,5/12</td>
</tr>
<tr>
<td>(6) 2</td>
<td>1/3,y,5/12</td>
</tr>
<tr>
<td>(7) T^+</td>
<td>1/3,1/3,1/3</td>
</tr>
<tr>
<td>(7) 1/3,1/3,1/3</td>
<td>1/3,1/3,1/3</td>
</tr>
<tr>
<td>(8) 3'</td>
<td>1/3,-1/3,z</td>
</tr>
<tr>
<td>(8) 3'</td>
<td>1/3,-1/3,z</td>
</tr>
<tr>
<td>(9) 3'</td>
<td>1/3,2/3,1/3</td>
</tr>
<tr>
<td>(9) 3'</td>
<td>1/3,2/3,1/3</td>
</tr>
<tr>
<td>(10) g'</td>
<td>x+1/2,x,z</td>
</tr>
<tr>
<td>(10) g'</td>
<td>x+1/2,x,z</td>
</tr>
<tr>
<td>(11) g'</td>
<td>1/6,1/3,5/6</td>
</tr>
<tr>
<td>(11) g'</td>
<td>1/6,1/3,5/6</td>
</tr>
<tr>
<td>(12) g'</td>
<td>2/3,1/3,5/6</td>
</tr>
<tr>
<td>(12) g'</td>
<td>2/3,1/3,5/6</td>
</tr>
</tbody>
</table>

**For (1/3,2,3/3) + set**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t</td>
<td>(1/3,2,3/3)</td>
</tr>
<tr>
<td>(1) 1/3,2,3/3</td>
<td>1/3,2,3/3</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>0,0,2/3</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>0,1/3,z</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>0,0,2/3</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>0,1/3,z</td>
</tr>
<tr>
<td>(4) 2</td>
<td>x,x+1/6,1/12</td>
</tr>
<tr>
<td>(4) 2</td>
<td>x,1/3,1/12</td>
</tr>
<tr>
<td>(5) 2</td>
<td>1/2,1/3,1/2</td>
</tr>
<tr>
<td>(5) 2</td>
<td>1/2,1/3,1/2</td>
</tr>
<tr>
<td>(6) 2</td>
<td>0,1/2,0</td>
</tr>
<tr>
<td>(6) 2</td>
<td>1/6,y,1/12</td>
</tr>
<tr>
<td>(7) T^+</td>
<td>1/3,1/3,1/3</td>
</tr>
<tr>
<td>(7) 1/3,1/3,1/3</td>
<td>1/3,1/3,1/3</td>
</tr>
<tr>
<td>(8) 3'</td>
<td>2/3,1/3,z</td>
</tr>
<tr>
<td>(8) 3'</td>
<td>2/3,1/3,z</td>
</tr>
<tr>
<td>(9) 3'</td>
<td>-1/3,1/3,z</td>
</tr>
<tr>
<td>(9) 3'</td>
<td>-1/3,1/3,z</td>
</tr>
<tr>
<td>(10) g'</td>
<td>x+1/2,x,z</td>
</tr>
<tr>
<td>(10) g'</td>
<td>x+1/2,x,z</td>
</tr>
<tr>
<td>(11) g'</td>
<td>1/3,2,3/3,1/6</td>
</tr>
<tr>
<td>(11) g'</td>
<td>1/3,2,3/3,1/6</td>
</tr>
<tr>
<td>(12) g'</td>
<td>1/3,2,3/3,1/6</td>
</tr>
<tr>
<td>(12) g'</td>
<td>1/3,2,3/3,1/6</td>
</tr>
</tbody>
</table>

### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td></td>
</tr>
<tr>
<td>(2/3,1/3,1/3) +</td>
<td></td>
</tr>
<tr>
<td>(1/3,2,3/3) +</td>
<td></td>
</tr>
</tbody>
</table>
Continued

| 36 | f | 1 | (1) x,y,z [u,v,w] | (2) y,x-y,z [v,u-v,w] | (3) x+y,x,z [u+v,u,w] |
| (4) y,x,z+1/2 [v,u-w] | (5) x-y,y,z+1/2 [u-v,v,w] | (6) x,x+y,z+1/2 [u,u+v,w] |
| (7) x,y,z [u,v,w] | (8) y,x+y,z [v,u+v,w] | (9) x-y,x,z [u-v,u,w] |
| (10) y,x,z+1/2 [v,u,w] | (11) x+y,y,z+1/2 [u+v,v,w] | (12) x,x-y,z+1/2 [u,u-v,w] |

| 18 | e | .2 | x,0,1/4 [u,0,0] | 0,x,1/4 [0,u,0] | x,x,1/4 [u,u,0] |
| (x,0,3/4 [u,0,0] | 0,x,3/4 [0,u,0] | x,x,3/4 [u,u,0] |

| 18 | d | 1/2,0,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

| 12 | c | 3. | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z+1/2 [0,0,w] |
| 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |

| 6 | b | 32 | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
\[ \mathbf{a}^* = (2\mathbf{a} + \mathbf{b})/3 \]  
Origin at 0,0,z

Along [1,0,0] p211  
\[ \mathbf{a}^* = (2\mathbf{a} + 4\mathbf{b} + \mathbf{c})/6 \]  
\[ \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \]  
Origin at x,0,0

Along [2,1,0] p2m'g'  
\[ \mathbf{a}^* = \mathbf{c}/3 \]  
\[ \mathbf{b}^* = \mathbf{b}/2 \]  
Origin at x,x/2,0
Origin on (3) at 3c'

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/12; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \]

Vertices

\[ \begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/12 & \quad 1/2,0,1/12 & \quad 2/3,1/3,1/12 & \quad 1/3,2/3,1/12 & \quad 0,1/2,1/12
\end{align*} \]
## Symmetry Operations

### For (0,0,0) + set

1. \([1] \quad (0,0,0)\)
2. \([2] \quad 0,0,z\)
3. \([3] \quad 0,0,z\)
4. \([4] \quad x,x,1/4\)
5. \([5] \quad x,0,1/4\)
6. \([6] \quad 0,y,1/4\)
7. \([7] \quad \bar{T}\)
8. \([8] \quad 0,0,z; 0,0,0\)
9. \([9] \quad 0,0,z; 0,0,0\)
10. \([10] \quad c' (0,0,1/2)\)

### For (2/3,1/3,1/3) + set

1. \([1] \quad (2/3,1/3,1/3)\)
2. \([2] \quad (0,0,1/3)\)
3. \([3] \quad (0,0,1/3)\)
4. \([4] \quad (1/2,1/2,0)\)
5. \([5] \quad (1/2,0,0)\)
6. \([6] \quad 1/3,y,5/12\)
7. \([7] \quad \bar{T}\)
8. \([8] \quad 1/3,-1/3,z; 1/3,-1/3,1/3\)
9. \([9] \quad 1/3,2/3,z; 1/3,2/3,1/3\)
10. \([10] \quad g' (-1/6,1/6,1/6)\)

### For (1/3,2/3,2/3) + set

1. \([1] \quad (1/3,2/3,2/3)\)
2. \([2] \quad (0,0,2/3)\)
3. \([3] \quad (0,0,2/3)\)
4. \([4] \quad (1/2,1/2,0)\)
5. \([5] \quad x,1/3,1/12\)
6. \([6] \quad 0,1/2,0\)
7. \([7] \quad \bar{T}\)
8. \([8] \quad 2/3,1/3,1/3\)
9. \([9] \quad -1/3,1/3,1/3\)
10. \([10] \quad g' (1/3,2/3,1/6)\)

### Generators selected

1; \(t(1,0,0); t(0,1,0); t(0,0,1); t(2/3,1/3,1/3); t(2); \(4); (7)\).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0))</td>
<td>((2/3,1/3,1/3))</td>
</tr>
</tbody>
</table>
Continued

36 f 1 (1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w] (4) y,x,z+1/2 [v,u,w] (5) x-y,y,z+1/2 [u+v,v,w] (6) x,x+y,z+1/2 [u,u-v,w] (7) x,y,z [u,v,w] (8) y,x+y,z [v,u-v,w] (9) x-y,x,z [u+v,u,w] (10) y,x,z+1/2 [v,u,w] (11) x+y,y,z+1/2 [u+v,v,w] (12) x,x-y,z+1/2 [u,u-v,w]

18 e .2' x,0,1/4 [u,2u,w] 0,x,1/4 [2u,u,w] x,x,1/4 [u,u,w] x,0,3/4 [u,2u,w] 0,x,3/4 [2u,u,w] x,x,3/4 [u,u,w]

18 d 1 1/2,0,0 [u,v,w] 0,1/2,0 [v,u-v,w] 1/2,1/2,0 [u+v,u,w] 0,1/2,1/2 [v,u,w] 1/2,0,1/2 [u+v,v,w] 1/2,1/2,1/2 [u,u-v,w]

12 c 3. 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w] 0,0,z+1/2 [0,0,w] 0,0,z+1/2 [0,0,w]

6 b 3. 0,0,0 [0,0,w] 0,0,1/2 [0,0,w] 0,0,1/2 [0,0,w]

6 a 32' 0,0,1/4 [0,0,w] 0,0,3/4 [0,0,w]

Symmetry of Special Projections

Along [0,0,1] p6'm'm
\[ a^* = (2a + b)/3 \quad b^* = (-a + b)/3 \]
Origin at 0,0,z

Along [1,0,0] p 2'11
\[ a^* = (2a + 4b + c)/6 \quad b^* = (a + 2b)/2 \]
Origin at x,0,0

Along [2,1,0] p2'mg'
\[ a^* = c/3 \quad b^* = b/2 \]
Origin at x,x/2,0
Origin on 6

Asymmetric unit: 
- $0 \leq x \leq 2/3$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1$; $x \leq (1+y)/2$; $y \leq \min(1-x,x)$

Vertices:
- $0,0,0$
- $0,0,1$
- $1/2,0,0$
- $1/2,0,1$
- $2/3,1/3,0$
- $2/3,1/3,1$

Symmetry Operations:

(1) $1$

(2) $3^* 0,0,z$

(3) $3^- 0,0,z$

(4) $2 0,0,z$

(5) $6^- 0,0,z$

(6) $6^+ 0,0,z$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>d</th>
<th>1</th>
<th>x,y,z [u,v,w]</th>
<th>y,x-y,z [v,u-v,w]</th>
<th>(3) x+y, x+z [u+v,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Positions</td>
<td>(4)</td>
<td>x, y, z [u, v, w]</td>
<td>(5) y, x+y, z [v, u+v, w]</td>
<td>(6) x-y, x, z [u-v,u,w]</td>
<td></td>
</tr>
<tr>
<td>Positions</td>
<td>3</td>
<td>c</td>
<td>1/2,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>Positions</td>
<td>2</td>
<td>b</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>Positions</td>
<td>1</td>
<td>a</td>
<td>0,0,z [0,0,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  
Origin at 0,0,z

Along [1,0,0] p1m'1  
\[ \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \]  
Origin at x,0,0

Along [2,1,0] p1m'1  
\[ \mathbf{a}^* = \mathbf{b}/2 \quad \mathbf{b}^* = \mathbf{c} \]  
Origin at x,x/2,0
Origin on 61'

Asymmetric unit

\[
\begin{align*}
0 & \leq x \leq 2/3; \\
0 & \leq y \leq 1/2; \\
0 & \leq z \leq 1; \\
x & \leq (1+y)/2; \\
y & \leq \min(1-x,x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1 & \quad 1/2,1/2,1
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1,0,0,0) \\
(2) & \quad 3^* \quad 0,0,z \\
& \quad (3z,0,0,0) \\
(3) & \quad 3' \quad 0,0,z \\
& \quad (3z^{-1},0,0,0)
\end{align*}
\]

For 1' + set

\[
\begin{align*}
(1) & \quad 1' \\
& \quad (1,0,0,0)' \\
(2) & \quad 3^{*'} \quad 0,0,z \\
& \quad (3z,0,0,0)' \\
(3) & \quad 3' \quad 0,0,z \\
& \quad (3z^{-1},0,0,0)'
\end{align*}
\]

\[
\begin{align*}
(4) & \quad 2' \quad 0,0,z \\
& \quad (2z,0,0,0)' \\
(5) & \quad 6' \quad 0,0,z \\
& \quad (6z^{-1},0,0,0)' \\
(6) & \quad 6' \quad 0,0,z \\
& \quad (6z,0,0,0)'
\end{align*}
\]
**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>d</td>
<td>11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) y,x-y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) y,x+y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(6) x-y,x,z [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>2..1'</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,1/2,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>3..1'</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>6..1'</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1] p61'**
  - Origin at 0,0,z
- **Along [1,0,0] p1m11'**
  - $a^* = a$, $b^* = b$
  - $a^* = (a + 2b)/2$, $b^* = c$
- **Along [2,1,0] p1m11'**
  - $a^* = b/2$, $b^* = c$
  - Origin at x,x/2,0
Origin on 6'

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1 & \quad 1/2,1/2,1
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \quad (3z \quad 0,0,0) \\
(3) & \quad 3^* \quad 0,0,z \quad (3z^{-1} \quad 0,0,0) \\
(4) & \quad 2' \quad 0,0,z \quad (2z \quad 0,0,0)' \\
(5) & \quad 6' \quad 0,0,z \quad (6z^{-1} \quad 0,0,0)' \\
(6) & \quad 6' \quad 0,0,z \quad (6z \quad 0,0,0)' \\
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x-y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>3 c 2'..</td>
<td>1/2,0,z [u,v,0]</td>
<td>0,1/2,z [v,u-v,0]</td>
</tr>
<tr>
<td></td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>1 a 6'..</td>
<td>0,0,z [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'  
\( a^* = a \quad b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p1m1  
\( a^* = (a + 2b)/2 \quad b^* = c \)  
Origin at x,0,0

Along [2,1,0] p1m1  
\( a^* = b/2 \quad b^* = c \)  
Origin at x,x/2,0
Origin on 6

Asymmetric unit

\[0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x)\]

Vertices

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Z</th>
<th>X'</th>
<th>Y'</th>
<th>Z'</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
<td>1/2,1/2,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,0,1</td>
<td>1/2,0,1</td>
<td>2/3,1/3,1</td>
<td>1/2,1/2,1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

For \(0,0,0\) + set

(1) 1

(2) 3 \cdot 0,0,z

(3) 3^-1 \cdot 0,0,z

(4) 2 \cdot 0,0,z

(5) 6 \cdot 0,0,z

(6) 6^-1 \cdot 0,0,z

For \(0,0,1\) + set

(1) t' \cdot (0,0,1)

(2) 3^-1 \cdot (0,0,1)' 0,0,z

(3) 3 \cdot (0,0,1)' 0,0,z

(4) 2' \cdot (0,0,1) 0,0,z

(5) 6^-1 \cdot (0,0,1)' 0,0,z

(6) 6 \cdot (0,0,1) 0,0,z
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>6</td>
</tr>
</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>(0,0,0) + (0,0,1)' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) y,x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td>(6) x-y,x,z [u-v,u,w]</td>
</tr>
</tbody>
</table>

| 1/2,0,z [0,0,w] |
| 0,1/2,z [0,0,w] |
| 1/2,1/2,z [0,0,w] |
| 1/3,2/3,z [0,0,w] |
| 2/3,1/3,z [0,0,w] |

Symmetry of Special Projections

Along [0,0,1] p61'  
\( \mathbf{a}^* = \mathbf{a} \)  
\( \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0] p2b 1m1  
\( \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2 \)  
\( \mathbf{b}^* = \mathbf{c} \)  
Origin at x,0,0

Along [2,1,0] p2b 1m1  
\( \mathbf{a}^* = \mathbf{b}/2 \)  
\( \mathbf{b}^* = \mathbf{c} \)  
Origin at x,x/2,0
Origin on 6'

**Asymmetric unit**

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1; \quad x \leq \frac{1+y}{2}; \quad y \leq \min(1-x,x) \]

**Vertices**

- \( 0,0,0 \)
- \( \frac{1}{2},0,0 \)
- \( \frac{2}{3},\frac{1}{3},0 \)
- \( \frac{1}{2},\frac{1}{2},0 \)
- \( 0,0,1 \)
- \( \frac{1}{2},0,1 \)
- \( \frac{2}{3},\frac{1}{3},1 \)
- \( \frac{1}{2},\frac{1}{2},1 \)

**Symmetry Operations**

For \((0,0,0)\) + set

1. \( 1 \)
2. \( 3^* \) 0,0,z
   - \( 3_z(0,0,0) \)
3. \( 3^-\) 0,0,z
   - \( 3_z^{-1}(0,0,0) \)
4. \( 2^* \) 0,0,z
   - \( 2_z(0,0,0)' \)
5. \( 6^* \) 0,0,z
   - \( 6_z(0,0,0)' \)
6. \( 6^-\) 0,0,z
   - \( 6_z^{-1}(0,0,0)' \)

For \((0,0,1)\)' + set

1. \( t' \) (0,0,1)
   - \( (0,0,1)' \)
2. \( 3^* \) (0,0,1)
   - \( 3_z(0,0,1)' \)
3. \( 3^-\) (0,0,1)
   - \( 3_z^{-1}(0,0,1)' \)
4. \( 2^* \) (0,0,1)
   - \( 2_z(0,0,1)' \)
5. \( 6^* \) (0,0,1)
   - \( 6_z(0,0,1)' \)
6. \( 6^-\) (0,0,1)
   - \( 6_z^{-1}(0,0,1)' \)
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)’ +</td>
<td>(2) y,x-y,z [v-u,v,w]</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td></td>
<td>(5) y,x+y,z [v-u-v,w]</td>
<td>(6) x-y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td>6 c 2’..</td>
<td>1/2,0,z [u,v,0]</td>
<td></td>
<td>0,1/2,z [v-u-v,0]</td>
<td>1/2,1/2,z [u+v,u,0]</td>
</tr>
<tr>
<td>4 b 3..</td>
<td>1/3,2/3,z [0,0,w]</td>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>2 a 6’..</td>
<td>0,0,z [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p61’
\[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] \( \mathbf{p}_{2b} \), 1m1
\[ \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2, \quad \mathbf{b}^* = \mathbf{c} \]
Origin at x,0,0

Along [2,1,0] \( \mathbf{p}_{2b} \), 1m1
\[ \mathbf{a}^* = b/2, \quad \mathbf{b}^* = c \]
Origin at x,x/2,0
Origin on 6₁

Asymmetric unit  
\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{6}\]

Vertices  
\[0,0,0\]  \[1,0,0\]  \[1,1,0\]  \[0,1,0\]  
\[0,0,\frac{1}{6}\]  \[1,0,\frac{1}{6}\]  \[1,1,\frac{1}{6}\]  \[0,1,\frac{1}{6}\]

Symmetry Operations

(1) 1  
(1 | 0,0,0)

(2) \(3^*\) (0,0,1/3) 0,0,z  
(3) \(3^*\) (0,0,2/3) 0,0,z

(3) \(3^*\) (0,0,1/3) 0,0,z  
(3) \(3^*\) (0,0,2/3) 0,0,z

(4) 2 (0,0,1/2) 0,0,z  
(2 | 0,0,1/2)

(5) 6' (0,0,5/6) 0,0,z  
(6) 6' (0,0,1/6) 0,0,z

(6) 6' (0,0,5/6) 0,0,z  
(6) 6' (0,0,1/6)
Generators selected

(1) t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>a</td>
</tr>
<tr>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) ( y ),x-y,z+1/3 [( v ),u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) ( x+y ),x,z+2/3 [( u+v ),u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) ( x ),y,z+1/2 [( u ),v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+( y ),z+5/6 [v,( u+v ),w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z+1/6 [( u-v ),u,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) p6  Along \([1,0,0]\) p1\( g'1\)  Along \([2,1,0]\) p1\( g'1\)

\( a^* = a \quad b^* = b \quad a^* = (a + 2b)/2 \quad b^* = c \quad a^* = b/2 \quad b^* = c \)

Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
**Origin** on 6,1'

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{6} \]

**Vertices**

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1,0,0</th>
<th>1,1,0</th>
<th>0,1,0</th>
<th>0,0,1/6</th>
<th>1,0,1/6</th>
<th>1,1,1/6</th>
<th>0,1,1/6</th>
</tr>
</thead>
</table>

**Symmetry Operations**

**For 1 + set**

1. \(1\) (1,0,0)
2. \(3^* (0,0,1/3) \quad 0,0,z\)
3. \(3^{-1} (0,0,2/3) \quad 0,0,z\)
4. \(2 (0,0,1/2) \quad 0,0,z\)
5. \(6^{-1} (0,0,5/6) \quad 0,0,z\)
6. \(6 (0,0,1/6) \quad 0,0,z\)

**For 1' + set**

1. \(1' (0,0,0)\)
2. \(3^* (0,0,1/3) \quad 0,0,z\)
3. \(3^{-1} (0,0,2/3) \quad 0,0,z\)
4. \(2' (0,0,1/2) \quad 0,0,z\)
5. \(6^{-1} (0,0,5/6) \quad 0,0,z\)
6. \(6' (0,0,1/6) \quad 0,0,z\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>a</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z+1/3</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z+2/3</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z+5/6</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z+1/6</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]  p61'  Along [1,0,0]  p1g11'  Along [2,1,0]  p1g11'
\( a^* = a \)  \( b^* = b \)  \( a^* = (a + 2b)/2 \)  \( b^* = c \)  \( a^* = b/2 \)  \( b^* = c \)

Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
Origin on 6,

Asymmetric unit

\begin{align*}
\text{Vertices} & \quad 0,0,0 & 1,0,0 & 1,1,0 & 0,1,0 \\
& \quad 0,0,1/6 & 1,0,1/6 & 1,1,1/6 & 0,1,1/6
\end{align*}

Symmetry Operations

\begin{align*}
(1) \quad & 1 \\
& (1 \mid 0,0,0) \\
(2) \quad & 3^* (0,0,1/3) \ 0,0,z \\
& (3_z^* 0,0,1/3) \\
(3) \quad & 3^* (0,0,2/3) \ 0,0,z \\
& (3_z^* 0,0,2/3) \\
(4) \quad & 2' (0,0,1/2) \ 0,0,z \\
& (2_z' 0,0,1/2)^* \\
(5) \quad & 6^* (0,0,5/6) \ 0,0,z \\
& (6_z^* 0,0,5/6)^* \\
(6) \quad & 6^* (0,0,1/6) \ 0,0,z \\
& (6_z^* 0,0,1/6)^*
\end{align*}
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 a 1</td>
<td>(1) ( x,y,z ) ([u,v,w]) (2) ( \bar{y},x-y,z+1/3 ) ([\bar{v},u-v,w]) (3) ( \bar{x}+y,\bar{x},z+2/3 ) ([\bar{u}+v,\bar{u},w]) (4) ( \bar{x},y,z+1/2 ) ([u,v,\bar{w}]) (5) ( y,x+y,z+3/6 ) ([v,u-v,w]) (6) ( x-y,x,z+1/6 ) ([u+v,\bar{u},\bar{w}])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \( p6' \) Along \([1,0,0]\) \( p1g1 \) Along \([2,1,0]\) \( p1g1 \)

\( a^* = a \) \( b^* = b \) \( a^* = (a+2b)/2 \) \( b^* = c \) \( a^* = b/2 \) \( b^* = c \)

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
Origin on $6_5$

Asymmetric unit: $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6$

Vertices:
- $0,0,0$
- $1,0,0$
- $1,1,0$
- $0,1,0$
- $0,0,1/6$
- $1,0,1/6$
- $1,1,1/6$
- $0,1,1/6$

Symmetry Operations:

1. $1$
2. $3^* (0,0,2/3) \quad 0,0,z$
3. $3^* (0,0,1/3) \quad 0,0,z$
4. $2 (0,0,1/2) \quad 0,0,z$
5. $6^* (0,0,1/6) \quad 0,0,z$
6. $6^* (0,0,5/6) \quad 0,0,z$

$P6_5$

170.1.1347

Hexagonal
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4)\).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 a 1</td>
<td>(1) (x,y,z) ([u,v,w])</td>
</tr>
<tr>
<td></td>
<td>(2) (y,x-y,z+2/3) ([v,u-v,w])</td>
</tr>
<tr>
<td></td>
<td>(3) (x+y,x,z+1/3) ([u+v,u,w])</td>
</tr>
<tr>
<td></td>
<td>(4) (x,y,z+1/2) ([u,v,w])</td>
</tr>
<tr>
<td></td>
<td>(5) (y,x+y,z+1/6) ([v,u+v,w])</td>
</tr>
<tr>
<td></td>
<td>(6) (x-y,x,z+5/6) ([u-v,u,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along ([0,0,1])</th>
<th>p6</th>
<th>Along ([1,0,0])</th>
<th>p1g'1</th>
<th>Along ([2,1,0])</th>
<th>p1g'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = (a + 2b)/2)</td>
<td>(b^* = c)</td>
<td>(a^* = b/2)</td>
<td>(b^* = c)</td>
</tr>
<tr>
<td>Origin at (0,0,z)</td>
<td>Origin at (x,0,0)</td>
<td>Origin at (x,x/2,0)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on $6_3 1'$

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 & \quad 0,1,0 \\
0,0,1/6 & \quad 1,0,1/6 & \quad 1,1,1/6 & \quad 0,1,1/6
\end{align*}
\]

Symmetry Operations

For \(1 \) + set

\[
\begin{align*}
(1) \quad & 1 \\
(1) & (1,0,0) \\
(2) & 3^+ (0,0,2/3) \quad 0,0,z \\
(3) & 3^- (0,0,1/3) \quad 0,0,z \\
(4) & 2 (0,0,1/2) \quad 0,0,z \\
(4) & (2_z,0,0,1/2) \\
(5) & 6^- (0,0,1/6) \quad 0,0,z \\
(5) & (6_z^{-1},0,0,1/6) \\
(6) & 6^+ (0,0,5/6) \quad 0,0,z \\
(6) & (6_z,0,0,5/6)
\end{align*}
\]

For \(1' \) + set

\[
\begin{align*}
(1) \quad & 1' \\
(1) & (1,0,0)' \\
(2) & 3^+ '(0,0,2/3) \quad 0,0,z \\
(3) & 3^- '(0,0,1/3) \quad 0,0,z \\
(4) & 2'(0,0,1/2) \quad 0,0,z \\
(4) & (2_z',0,0,1/2) \\
(5) & 6^- '(0,0,1/6) \quad 0,0,z \\
(5) & (6_z^{-1}',0,0,1/6) \\
(6) & 6^+ '(0,0,5/6) \quad 0,0,z \\
(6) & (6_z,0,0,5/6)'
\end{align*}
\]

170.2.1348 - 1 - 2933
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 a 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) y,-x-y,z+2/3 [0,0,0]</td>
<td>(3) x+y,x,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [0,0,0]</td>
<td>(5) y,x+y,z+1/6 [0,0,0]</td>
<td>(6) x-y,x,z+5/6 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p61'  
\( a^* = a \)  \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p1g11'  
\( a^* = (a+2b)/2 \)  \( b^* = c \)  
Origin at x,0,0

Along [2,1,0] p1g11'  
\( a^* = b/2 \)  \( b^* = c \)  
Origin at x,x/2,0
Origin on $6_5'$

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq 1$; $0 \leq z \leq 1/6$

Vertices

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices</td>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
</tr>
<tr>
<td></td>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
</tr>
</tbody>
</table>

Symmetry Operations

1. $1$
   $1$ $1$
   $1$ $1$

2. $3^*$ $(0,0,2/3)$ $0,0,z$
   $3^*$ $(0,0,2/3)$ $0,0,z$

3. $3^*$ $(0,0,1/3)$ $0,0,z$
   $3^*$ $(0,0,1/3)$ $0,0,z$

4. $2' (0,0,1/2)$ $0,0,z$
   $2' (0,0,1/2)$ $0,0,z$

5. $6' (0,0,1/6)$ $0,0,z$
   $6' (0,0,1/6)$ $0,0,z$

6. $6' (0,0,5/6)$ $0,0,z$
   $6' (0,0,5/6)$ $0,0,z$
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>a</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) x+y, x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) x, y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) y,x+y,z+1/6 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(6) x-y,x,z+5/6 [u+v,u,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6'</th>
<th>Along [1,0,0]</th>
<th>p1g1</th>
<th>Along [2,1,0]</th>
<th>p1g1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a</td>
<td>b' = b</td>
<td>a' = (a + 2b)/2</td>
<td>b' = c</td>
<td>a' = b/2</td>
<td>b' = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2 on 6

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{3}; \quad y \leq x \]

Vertices

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1,0,0</th>
<th>1,1,0</th>
<th>0,0,1/3</th>
<th>1,0,1/3</th>
<th>1,1,1/3</th>
</tr>
</thead>
</table>

Symmetry Operations

- \( (1) 1 \)
- \( (1 | 0,0,0) \)
- \( (2) 3^* (0,0,2/3) \)
- \( (3) 3^* (0,0,1/3) \)
- \( (3 z^* 0,0,2/3) \)
- \( (3 z^* 0,0,1/3) \)

- \( (4) 2 0,0,z \)
- \( (2_z | 0,0,0) \)
- \( (5) 6^* (0,0,2/3) \)
- \( (6) 6^* (0,0,1/3) \)
- \( (6 z^* 0,0,2/3) \)
- \( (6 z^* 0,0,1/3) \)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

| 6 | c | 1 | (1) x,y,z [u,v,w] | (2) \(\bar{y},x-y,z+2/3\) [v,\(u-v,w\)] | (3) \(x+y,\bar{x},z+1/3\) [\(u+v,\bar{u},w\)] |
| 3 | b | 2.. | 1/2,1/2,z [0,0,w] | 1/2,0,z+2/3 [0,0,w] | 0,1/2,z+1/3 [0,0,w] |
| 3 | a | 2.. | 0,0,z [0,0,w] | 0,0,z+2/3 [0,0,w] | 0,0,z+1/3 [0,0,w] |

Symmetry of Special Projections

Along [0,0,1] p6  Along [1,0,0] p1m'1  Along [2,1,0] p1m'1
\(a^* = a\)  \(b^* = b\)  \(a^* = b/2\)  \(b^* = c\)
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0

Continued
Origin on $21'$ on $6_21'$

Asymmetric unit

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x\]

Vertices

\[\begin{array}{ccc}
0,0,0 & 1,0,0 & 1,1,0 \\
0,0,1/3 & 1,0,1/3 & 1,1,1/3
\end{array}\]

Symmetry Operations

For $1' +$ set

\[
\begin{align*}
(1) & \quad 1 & & (2) & \quad 3' \ (0,0,2/3) & \quad 0,0,z \\
& (1|0,0,0) & & (3_z|0,0,2/3) & & (3_z|0,0,1/3) \\
(4) & \quad 2 \quad 0,0,z & & (5) & \quad 6' \ (0,0,2/3) & \quad 0,0,z \\
& (2_z|0,0,0) & & (6_z^{-1}|0,0,2/3) & & (6_z|0,0,1/3)
\end{align*}
\]

For $1' -$ set

\[
\begin{align*}
(1) & \quad 1' & & (2) & \quad 3' \ (0,0,2/3) & \quad 0,0,z \\
& (1|0,0,0)' & & (3_z|0,0,2/3)' & & (3_z|0,0,1/3)' \\
(4) & \quad 2' \quad 0,0,z & & (5) & \quad 6' \ (0,0,2/3) & \quad 0,0,z \\
& (2_z|0,0,0)' & & (6_z^{-1}|0,0,2/3)' & & (6_z|0,0,1/3)'
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 11'</td>
<td></td>
<td></td>
<td>(1) x,y,z [0,0,0] (2) y,x-y,z+2/3 [0,0,0] (3) x+y, x,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td>3 b 2..1'</td>
<td></td>
<td></td>
<td>(4) x,y,z [0,0,0] (5) y,x+y,z+2/3 [0,0,0] (6) x-y, x,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td>3 a 2..1'</td>
<td></td>
<td></td>
<td>(7) x, y, z [0,0,0] (8) y,x+y, z+2/3 [0,0,0] (9) x-y, x,z+1/3 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1]  p6'  
  Origin at 0,0,z  
  \( a^* = a \)  \( b^* = b \)

- Along [1,0,0]  p1m1'  
  Origin at x,0,0  
  \( a^* = (a + 2b)/2 \)  \( b^* = c \)

- Along [2,1,0]  p1m1'  
  Origin at x,x/2,0  
  \( a^* = b/2 \)  \( b^* = c \)
Origin on 2' on 6'₁

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x \]

Vertices

\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 \\
0,0,1/3 & \quad 1,0,1/3 & \quad 1,1,1/3
\end{align*}

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(1') & \quad 0,0,0 \\
(2) & \quad 3' (0,0,2/3) \quad 0,0,z \\
(3) & \quad 3' (0,0,1/3) \quad 0,0,z \\
(4) & \quad 2' \ 0,0,z \\
(5) & \quad 6' \ 0,0,2/3 \quad 0,0,z \\
(6) & \quad 6' \ 0,0,1/3 \quad 0,0,z
\end{align*}
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

### Positions

<table>
<thead>
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<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>c</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z+2/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x-y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>2'. 1/2,1/2,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,0,z+2/3 [v,u-v,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,z+1/3 [u+v,u,0]</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>2'. 0,0,z [u,v,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+2/3 [v,u-v,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+1/3 [u+v,u,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p6'
  - Origin at 0,0,z
  - \( a^* = a \) \( b^* = b \)

- Along [1,0,0] p1m1
  - Origin at x,0,0
  - \( a^* = (a+2b)/2 \) \( b^* = c \)

- Along [2,1,0] p1m1
  - Origin at x,x/2,0
  - \( a^* = b/2 \) \( b^* = c \)
Origin on 2’ on 6_2

Asymmetric unit

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x\]

Vertices

\[\begin{array}{ccc}
0,0,0 & 1,0,0 & 1,1,0 \\
0,0,1/3 & 1,0,1/3 & 1,1,1/3 \\
\end{array}\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[\begin{array}{ccc}
(1) & 1 & (2) 3' (0,0,2/3) \quad 0,0,z \\
(1|0,0,0) & (3_z|0,0,2/3) & (3) 3' (0,0,1/3) \quad 0,0,z \\
(4) 2' 0,0,z & (5) 6' (0,0,2/3) \quad 0,0,z & (6) 6' (0,0,1/3) \quad 0,0,z \\
(2_z|0,0,0)' & (6_z^{-1}|0,0,2/3)' & (6_z|0,0,1/3) \\
\end{array}\]

For \((0,0,1)' + \text{set}\)

\[\begin{array}{ccc}
(1) t' (0,0,1) & (2) 3' (0,0,5/3) \quad 0,0,z & (3) 3' (0,0,4/3) \quad 0,0,z \\
(1|0,0,1)' & (3_z|0,0,5/3)' & (3_z^{-1}|0,0,4/3) \\
(4) 2 (0,0,1) 0,0,z & (5) 6' (0,0,5/3) \quad 0,0,z & (6) 6' (0,0,4/3) \quad 0,0,z \\
(2_z|0,0,1) & (6_z^{-1}|0,0,5/3) & (6_z|0,0,4/3)' \\
\end{array}\]

171.4.1353 - 1 - 2943
Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1) + (0,1,0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z+1/3 [u-v,u,w]</td>
<td>(3) x+y,x,z+1/3 [u-v,u,w]</td>
<td></td>
</tr>
<tr>
<td>6 b 2'..</td>
<td>1/2,1/2,z [u,v,0]</td>
<td>1/2,0,z+2/3 [v,u-v,0]</td>
<td>0,1/2,z+1/3 [u-v,u,0]</td>
</tr>
<tr>
<td>6 a 2'..</td>
<td>0,0,z [u,v,0]</td>
<td>0,0,z+2/3 [v,u-v,0]</td>
<td>0,0,z+1/3 [u-v,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p61'</th>
<th>Along [1,0,0]</th>
<th>p2b 1m'1</th>
<th>Along [2,1,0]</th>
<th>p2b' 1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = (a + 2b)/2, b* = c</td>
<td>a* = b/2, b* = c</td>
<td>a* = b/2, b* = c</td>
<td>a* = b/2, b* = c</td>
<td>a* = b/2, b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td>Origin at x,x/2,0</td>
<td>Origin at x,x/2,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin on 2' on 6_2'

Asymmetric unit

\[ \begin{align*}
0 \leq x \leq 1; & \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x \\
\end{align*} \]

Vertices

\[ \begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 \\
0,0,1/3 & \quad 1,0,1/3 & \quad 1,1,1/3 \\
\end{align*} \]

Symmetry Operations

For (0,0,0) + set

\[ \begin{align*}
(1) & \quad 1 \\
(1' | 0,0,0) & \quad (3^* | 0,0,2/3) \quad 0,0,z \\
(3 | 3^* | 0,0,2/3) & \quad (3_{z}^{-1} | 0,0,1/3) \\
(4) & \quad 2 \quad 0,0,z \\
(2_{z} | 0,0,0) & \quad (5^* | 0,0,2/3) \quad 0,0,z \\
(6 | 6^* | 0,0,2/3) & \quad (6_{z} | 0,0,1/3) \\
(5) & \quad 6^* \quad (0,0,2/3) \quad 0,0,z \\
(6_{z} | 0,0,1/3)' & \quad (6_{z} | 0,0,1/3) \\
(6) & \quad 6^* \quad (0,0,1/3) \quad 0,0,z \\
(6_{z} | 0,0,1/3)' & \quad (6_{z} | 0,0,1/3)' \\
\end{align*} \]

For (0,0,1)' + set

\[ \begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(1' | 0,0,1)' & \quad (2) \quad 3^* \quad (0,0,5/3) \quad 0,0,z \\
(3 | 3^* | 0,0,5/3)' & \quad (3_{z}^{-1} | 0,0,4/3) \\
(4) & \quad 2' \quad (0,0,1) \quad 0,0,z \\
(2_{z} | 0,0,1)' & \quad (5) \quad 6^* \quad (0,0,5/3) \quad 0,0,z \\
(6 | 6^* | 0,0,5/3)' & \quad (6_{z} | 0,0,4/3) \\
(6) & \quad 6^* \quad (0,0,4/3) \quad 0,0,z \\
(6_{z} | 0,0,4/3) & \quad (6_{z} | 0,0,4/3) \\
\end{align*} \]
Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0)+</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
<td>(0,0,1)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+1/3 [u-v,u+w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [v,u,v,w]</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>b 2..</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,0,z+2/3 [0,0,w]</td>
</tr>
<tr>
<td>6</td>
<td>a 2..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+2/3 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,0,z+1/3 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**  
  - **p61'**  
    - $a^* = a$  
    - $b^* = b$  
  - Origin at 0,0,z

- **Along [1,0,0]**  
  - **p2b, 1m1**  
    - $a^* = (a + 2b)/2$  
    - $b^* = c$  
  - Origin at x,0,0

- **Along [2,1,0]**  
  - **p2b, 1m1**  
    - $a^* = b/2$  
    - $b^* = c$  
  - Origin at x,x/2,0
**Origin** on 2 on 6

**Asymmetric unit**

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0 ≤ x ≤ 1;</th>
<th>0 ≤ y ≤ 1;</th>
<th>0 ≤ z ≤ 1/3;</th>
<th>y ≤ x</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0</td>
<td>0,0,0</td>
<td>0,0,0</td>
<td>0,0,0</td>
<td></td>
</tr>
<tr>
<td>0,1/3</td>
<td>0,0,1/3</td>
<td>0,0,1/3</td>
<td>0,1/3</td>
<td></td>
</tr>
<tr>
<td>1,0</td>
<td>1,0,0</td>
<td>1,0,0</td>
<td>1,0</td>
<td></td>
</tr>
<tr>
<td>1,1/3</td>
<td>1,0,1/3</td>
<td>1,0,1/3</td>
<td>1,1/3</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. $1$
2. $3^*$ (0,0,1/3) 0,0,z
3. $3^*$ (0,0,2/3) 0,0,z
4. $2$ 0,0,z
5. $6^*$ (0,0,1/3) 0,0,z
6. $6^*$ (0,0,2/3) 0,0,z

$1^*$ $0,0,0$
$3^*$ (0,0,1/3)
$3^*$ (0,0,2/3)
$2^*$ $0,0,0$
$6^*$ (0,0,1/3)
$6^*$ (0,0,2/3)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z+1/3 [v,u-v,w]</td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y,x+y,z+1/3 [v,u+v,w]</td>
<td>(6) x-y,x,z+2/3 [u-v,u,w]</td>
</tr>
<tr>
<td>3 b 2..</td>
<td>1/2,1/2,z [0,0,w]</td>
<td>1/2,0,z+1/3 [0,0,w]</td>
<td>0,1/2,z+2/3 [0,0,w]</td>
</tr>
<tr>
<td>3 a 2..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/3 [0,0,w]</td>
<td>0,0,z+2/3 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6</th>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
<th>Along [2,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (a + 2b)/2</td>
<td>b* = c</td>
<td>a* = b/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on 21' on 6_31'

**Asymmetric unit**

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 \\
0,0,1/3 & \quad 1,0,1/3 & \quad 1,1,1/3 \\
\end{align*}
\]

**Symmetry Operations**

For \(1 + \) set

1. \(\mathbf{1}\) \(\begin{pmatrix} 1 \end{pmatrix} \quad \begin{pmatrix} 0,0,0 \end{pmatrix}\)

2. \(\mathbf{3}^*\) \((0,0,1/3)\) \((0,0,z)\)

3. \(\mathbf{3}^*\) \((0,0,2/3)\) \((0,0,z)\)

4. \(\mathbf{2}\) \((0,0,z)\)

5. \(\mathbf{6}^*\) \((0,0,1/3)\) \((0,0,z)\)

6. \(\mathbf{6}^*\) \((0,0,2/3)\) \((0,0,z)\)

For \(1' + \) set

1. \(\mathbf{1}'\) \(\begin{pmatrix} 1 \end{pmatrix} \quad \begin{pmatrix} 0,0,0' \end{pmatrix}\)

2. \(\mathbf{3}^*\) \((0,0,1/3)\) \((0,0,z)\)

3. \(\mathbf{3}^*\) \((0,0,2/3)\) \((0,0,z)\)

4. \(\mathbf{2'}\) \((0,0,z)\)

5. \(\mathbf{6}^*\) \((0,0,1/3)\) \((0,0,z)\)

6. \(\mathbf{6}^*\) \((0,0,2/3)\) \((0,0,z)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4): 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) y,x-y,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td>3 b 2..1'</td>
<td>1/2,1/2,z [0,0,0]</td>
<td>1/2,0,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td>3 a 2..1'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/3 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p61'</th>
<th>Along [1,0,0]</th>
<th>p1m11'</th>
<th>Along [2,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a* = (a + 2b)/2</td>
<td>b* = c</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2' on 6'_4:

Asymmetric unit: $0 \leq x \leq 1; 0 \leq y \leq 1; 0 \leq z \leq 1/3; y \leq x$

Vertices:
- $0,0,0$
- $0,0,1/3$
- $0,1,0$
- $1,0,0$
- $1,0,1/3$
- $1,1,0$
- $1,1,1/3$

Symmetry Operations:

1. $1$
2. $3' (0,0,1/3) 0,0,z$
3. $3' (0,0,2/3) 0,0,z$
4. $2' 0,0,z$
5. $6' (0,0,1/3) 0,0,z$
6. $6' (0,0,2/3) 0,0,z$
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4). \)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>c</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6)</td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>2'..</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,0,z+1/3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,z+2/3</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>2'..</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+1/3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+2/3</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- Along \([0,0,1]\) p6'
  \( \mathbf{a}^* = \mathbf{a} \)  \( \mathbf{b}^* = \mathbf{b} \)
  Origin at \(0,0,z\)

- Along \([1,0,0]\) p1m1
  \( \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2 \)  \( \mathbf{b}^* = \mathbf{c} \)
  Origin at \(x,0,0\)

- Along \([2,1,0]\) p1m1
  \( \mathbf{a}^* = \mathbf{b}/2 \)  \( \mathbf{b}^* = \mathbf{c} \)
  Origin at \(x,x/2,0\)
Origin on 2 on 6'₄

Asymmetric unit

\begin{align*}
0 \leq x \leq 1; & \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/3; \quad y \leq x
\end{align*}

Vertices

\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 \\
0,0,1/3 & \quad 1,0,1/3 & \quad 1,1,1/3
\end{align*}

Symmetry Operations

For \((0,0,0) + \) set

\begin{align*}
(1) \ 1 & \quad (2) \ 3' \ (0,0,1/3) \quad 0,0,z \\
(1 \ 0,0,0) & \quad (3_z \ 0,0,1/3) & \quad (3_z \ 0,0,2/3)
\end{align*}

\begin{align*}
(4) \ 2 \ 0,0,z \\
(2_z \ 0,0,0) & \quad (5) \ 6' \ (0,0,1/3) \quad 0,0,z \\
& \quad (6_z^{-1} \ 0,0,1/3)
\end{align*}

For \((0,0,1)' + \) set

\begin{align*}
(1) \ t' \ (0,0,1) & \quad (2) \ 3' \ (0,0,4/3) \quad 0,0,z \\
(1 \ 0,0,1)' & \quad (3_z \ 0,0,4/3) & \quad (3_z \ 0,0,5/3)
\end{align*}

\begin{align*}
(4) \ 2' \ (0,0,1) \ 0,0,z \\
(2_z \ 0,0,1)' & \quad (5) \ 6' \ (0,0,4/3) \quad 0,0,z \\
& \quad (6_z^{-1} \ 0,0,4/3)
\end{align*}
Generators selected  (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

**Positions**

<table>
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<tr>
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<th>Wyckoff letter</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>c</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z+1/3 [v,u+v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z+1/3 [v,u-v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x-y,x,z+2/3 [u-v,u,w]</td>
<td></td>
</tr>
</tbody>
</table>

| 6            | b              | 1/2,1/2,z [0,0,w] | 1/2,0,z+1/3 [0,0,w] |
|              |                | 0,0,z [0,0,w] |
|              |                | 0,0,z+1/3 [0,0,w] |
|              |                | 0,0,z+2/3 [0,0,w] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p61'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p_{2b'} 1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a + 2b)/2</td>
<td></td>
</tr>
<tr>
<td>b* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p_{2b'} 1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b/2</td>
<td></td>
</tr>
<tr>
<td>b* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 2' on 6_4'

Asymmetric unit

\[ 0 < x < 1; \quad 0 < y < 1; \quad 0 < z < \frac{1}{3}; \quad y < x \]

Vertices

\[ 0,0,0 \quad 1,0,0 \quad 1,1,0 \]
\[ 0,0,\frac{1}{3} \quad 1,0,\frac{1}{3} \quad 1,1,\frac{1}{3} \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1\)
2. \(3' (0,0,1/3) \quad 0,0,z \quad (3_z | 0,0,1/3)'
3. \(3' (0,0,2/3) \quad 0,0,z \quad (3_z | 0,0,2/3)'
4. \(2' (0,0,0) \quad 0,0,z \quad (2_z | 0,0,0)'
5. \(6' (0,0,1/3) \quad 0,0,z \quad (6_z | 0,0,1/3)\)
6. \(6' (0,0,2/3) \quad 0,0,z \quad (6_z | 0,0,2/3)'

For \((0,0,1) + \) set

1. \(t' (0,0,1) \quad 0,0,z \quad (2_z | 0,0,1)'
2. \(3' (0,0,4/3) \quad 0,0,z \quad (3_z | 0,0,4/3)
3. \(3' (0,0,5/3) \quad 0,0,z \quad (3_z | 0,0,5/3)'
4. \(2 (0,0,1) \quad 0,0,z \quad (2_z | 0,0,1)
5. \(6' (0,0,4/3) \quad 0,0,z \quad (6_z | 0,0,4/3)'
6. \(6' (0,0,5/3) \quad 0,0,z \quad (6_z | 0,0,5/3)\)
Generators selected \( (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4). \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 12 \ c \ 1 ) ((0,0,0) + (0,0,1)' + ) ( (0,0,0) + (0,0,1)' + )</td>
<td></td>
</tr>
<tr>
<td>( (1) \ x,y,z \ [u,v,w] ) ( (2) \ y,\overline{x-y},z+1/3 \ [v,\overline{u+v},\overline{w}] ) ( (3) \ x+y,\overline{x},z+2/3 \ [\overline{u+v},\overline{u},w] )</td>
<td></td>
</tr>
<tr>
<td>( (4) \ \overline{x},\overline{y},z \ [u,v,w] ) ( (5) \ y,x+y,z+1/3 \ [v,\overline{u+v},\overline{w}] ) ( (6) \ x-y,x,z+2/3 \ [\overline{u+v},\overline{u},w] )</td>
<td></td>
</tr>
<tr>
<td>( 6 \ b \ 2') ( 1/2,1/2,z \ [u,v,0] ) ( 1/2,0,z+1/3 \ [v,\overline{u+v},0] ) ( 0,1/2,z+2/3 \ [\overline{u+v},\overline{u},0] )</td>
<td></td>
</tr>
<tr>
<td>( 6 \ a \ 2') ( 0,0,z \ [u,v,0] ) ( 0,0,z+1/3 \ [v,\overline{u+v},0] ) ( 0,0,z+2/3 \ [\overline{u+v},\overline{u},0] )</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \( p61' \)
\( a^* = a \ b^* = b \)
Origin at \(0,0,z\)

Along \([1,0,0]\) \( p_{2b'} \ 1m1 \)
\( a^* = (a + 2b)/2 \ b^* = c \)
Origin at \(x,0,0\)

Along \([2,1,0]\) \( p_{2b'} \ 1m1 \)
\( a^* = b/2 \ b^* = c \)
Origin at \(x,x/2,0\)
Origin on 3 on 6

Asymmetric unit:

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x < (1 + y)/2; \quad y \leq \min(1 - x, (1 + x)/2) \]

Vertices:

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2 & \quad 0,1/2,1/2
\end{align*}
\]

Symmetry Operations:

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 1 \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^* \quad 0,0,z \\
(4) & \quad 2 \quad 0,0,1/2 \\
(2) & \quad 0,0,1/2 \\
(5) & \quad 6 \quad (0,0,1/2) \quad 0,0,z \\
(6) & \quad 6^* \quad (0,0,1/2) \quad 0,0,z \\
(6) & \quad (0,0,1/2)
\end{align*}
\]
Continued

Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) ( x,y,z [u,v,w] ) (2) ( y,x-y,z [v,u-v,w] ) (3) ( x+y,x,z [u+v,u,w] ) (4) ( x,y,z+1/2 [u,v,w] )</td>
<td></td>
</tr>
<tr>
<td>2 b 3..</td>
<td>( 1/3,2/3,z [0,0,w] ) ( 2/3,1/3,z+1/2 [0,0,w] )</td>
<td></td>
</tr>
<tr>
<td>2 a 3..</td>
<td>( 0,0,z [0,0,w] ) ( 0,0,z+1/2 [0,0,w] )</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along \([0,0,1]\) \( p6 \) \( a^* = a \) \( b^* = b \) Origin at \( 0,0,z \)
Along \([1,0,0]\) \( p1g'1 \) \( a^* = (a + 2b)/2 \) \( b^* = c \) Origin at \( x,0,0 \)
Along \([2,1,0]\) \( p1g'1 \) \( a^* = b/2 \) \( b^* = c \) Origin at \( x,x/2,0 \)
**Origin** on 31' on 6_31'

**Asymmetric unit**

- $0 \leq x \leq 2/3$; $0 \leq y \leq 2/3$; $0 \leq z \leq 1/2$; $x \leq (1 + y)/2$; $y \leq \min(1 - x,(1 + x)/2)$

**Vertices**

- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/2$
- $1/2,0,1/2$
- $2/3,1/3,1/2$
- $1/3,2/3,1/2$
- $0,1/2,1/2$

**Symmetry Operations**

For 1 + set

1. $1$
   - $1$ on $(0,0,0)$
2. $3'$ on $0,0,z$
   - $(3_z | 0,0,0)$
3. $3'$ on $0,0,z$
   - $(3_z^{-1} | 0,0,0)$
4. $2$ on $(0,0,1/2)$
   - $(2_z | 0,0,1/2)$
   - $(6_z | 0,0,1/2)$
5. $6'$ on $(0,0,1/2)$
   - $(6_z^{-1} | 0,0,1/2)$
6. $6'$ on $(0,0,1/2)$
   - $(6_z | 0,0,1/2)$

For 1' + set

1. $1'$
   - $1'$ on $(0,0,0)'$
2. $3'$ on $0,0,z$
   - $(3_z | 0,0,0)'$
3. $3'$ on $0,0,z$
   - $(3_z^{-1} | 0,0,0)'$
4. $2'$ on $(0,0,1/2)$
   - $(2_z | 0,0,1/2)'$
   - $(6_z^{-1} | 0,0,1/2)'$
5. $6'$ on $(0,0,1/2)$
   - $(6_z^{-1} | 0,0,1/2)'$
6. $6'$ on $(0,0,1/2)$
   - $(6_z | 0,0,1/2)'$
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 11'</td>
<td>1 +</td>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) y - x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x + y,x,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z+1/2 [0,0,0]</td>
<td>(5) y,x+y,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 b 3..1'</td>
<td>1/3,2/3,z [0,0,0]</td>
<td>2/3,1/3,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2 a 3..1'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p61'  
\[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]  
Origin at 0,0,z

Along [1,0,0] p1g11'  
\[ \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2, \quad \mathbf{b}^* = \mathbf{c} \]  
Origin at x,0,0

Along [2,1,0] p1g11'  
\[ \mathbf{a}^* = \mathbf{b}/2, \quad \mathbf{b}^* = \mathbf{c} \]  
Origin at x,x/2,0
**Origin** on 3 on $6'_3$

**Asymmetric unit**

- $0 \leq x \leq 2/3$;
- $0 \leq y \leq 2/3$;
- $0 \leq z \leq 1/2$;
- $x \leq (1 + y)/2$;
- $y \leq \min(1 - x,(1 + x)/2)$

**Vertices**

- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/2$
- $1/2,0,1/2$
- $2/3,1/3,1/2$
- $1/3,2/3,1/2$
- $0,1/2,1/2$

**Symmetry Operations**

1. $1$
   - $(1 | 0,0,0)$
2. $3^*$ $0,0,z$
   - $(3_z | 0,0,0)$
3. $3^*$ $0,0,z$
   - $(3_{z}^{-1} | 0,0,0)$
4. $2' (0,0,1/2)$ $0,0,z$
   - $(2_z | 0,0,1/2)'$
5. $6' (0,0,1/2)$ $0,0,z$
   - $(6_z^{-1} | 0,0,1/2)'$
6. $6' (0,0,1/2)$ $0,0,z$
   - $(6_z | 0,0,1/2)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 c 1</td>
<td>(1) x,y,z [u,v,w] (2) y-x,y,z [v,u-v,w] (3) x+y,y,z [u+v,u,w] (4) x,y,z+1/2 [u,v,w] (5) y+x+y,z+1/2 [v,u-v,w] (6) x-y,x,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td>2 b 3..</td>
<td>1/3,2/3,z [0,0,w] 2/3,1/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 a 3..</td>
<td>0,0,z [0,0,w] 0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p6'</th>
<th>Along [1,0,0] p1g1</th>
<th>Along [2,1,0] p1g1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = (a + 2b)/2</td>
<td>a* = b/2 b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
**Origin on $\bar{6}$**

**Asymmetric unit**

$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$

**Vertices**

$0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0$

$0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2 \quad 1/3,2/3,1/2 \quad 0,1/2,1/2$

**Symmetry Operations**

1. \(1\)
2. \(3^+ \quad 0,0,z\)
3. \(3^- \quad 0,0,z\)
4. \(m \quad x,y,0\)
5. \(\bar{6}^- \quad 0,0,z; 0,0,0\)
6. \(\bar{6}^+ \quad 0,0,z; 0,0,0\)

\(\bar{6} \quad P\bar{6}\)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 l 1 (1) x,y,z [u,v,w]</td>
<td>(2) y-x,y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y-x,y,z [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td>3 k m.. x,y,1/2 [0,0,w]</td>
<td>y-x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x+y,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>3 j m.. x,y,0 [0,0,w]</td>
<td>y-x,y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x+y,x,0 [0,0,w]</td>
</tr>
<tr>
<td>2 i 3.. 2/3,1/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>2 h 3.. 1/3,2/3,z [0,0,w]</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>2 g 3.. 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1 f 6.. 2/3,1/3,1/2 [0,0,w]</td>
<td>2/3,1/3,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 e 6.. 2/3,1/3,0 [0,0,w]</td>
<td>2/3,1/3,0 [0,0,w]</td>
</tr>
<tr>
<td>1 d 6.. 1/3,2,1/2 [0,0,w]</td>
<td>1/3,2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 c 6.. 1/3,2,0 [0,0,w]</td>
<td>1/3,2,0 [0,0,w]</td>
</tr>
<tr>
<td>1 b 6.. 0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 a 6.. 0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31'  
a* = a  b* = b  
Origin at 0,0,z

Along [1,0,0] p1m1  
a* = c  b* = (a+2b)/2  
Origin at x,0,0

Along [2,1,0] p1m1  
a* = c  b* = b/2  
Origin at x,x/2,0
Origin on $\bar{6}1'$

Asymmetric unit

$0 \leq x \leq 2/3;\quad 0 \leq y \leq 2/3;\quad 0 \leq z \leq 1/2;\quad x \leq (1+y)/2;\quad y \leq \min(1-x,(1+x)/2)$

Vertices

$0,0,0\quad 1/2,0,0\quad 2/3,1/3,0\quad 1/3,2/3,0\quad 0,1/2,0$

$0,0,1/2\quad 1/2,0,1/2\quad 2/3,1/3,1/2\quad 1/3,2/3,1/2\quad 0,1/2,1/2$

Symmetry Operations

For $1 +$ set

(1) $1$

(1 $0,0,0$

(2) $3' \quad 0,0,z$

(3) $3' \quad 0,0,z$

(4) $m \quad x,y,0$

$m_z | 0,0,0$

(5) $\bar{6}' \quad 0,0,z; 0,0,0$

(6) $\bar{6}' \quad 0,0,z; 0,0,0$

For $1' +$ set

(1) $1'$

(1 $0,0,0'$

(2) $3' \quad 0,0,z$

(3) $3' \quad 0,0,z$

(4) $m' \quad x,y,0$

$m_z | 0,0,0'$

(5) $\bar{6}' \quad 0,0,z; 0,0,0$

(6) $\bar{6}' \quad 0,0,z; 0,0,0$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); 1'.

Positions

<table>
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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1'</td>
<td>(1) x,y,z [0,0,0] (2) y,x-y,z [0,0,0] (3) x+y,x,z [0,0,0] (4) x,y,z [0,0,0] (5) y,x-y,z [0,0,0] (6) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>6 l 11'</td>
<td>x,y,1/2 [0,0,0] y,x-y,1/2 [0,0,0] x+y,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 k m..1'</td>
<td>x,y,0 [0,0,0] y,x-y,0 [0,0,0] x+y,x,0 [0,0,0]</td>
</tr>
<tr>
<td>2 i 3..1'</td>
<td>2/3,1/3,z [0,0,0] 2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>2 h 3..1'</td>
<td>1/3,2/3,z [0,0,0] 1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>2 g 3..1'</td>
<td>0,0,z [0,0,0] 0,0,z [0,0,0]</td>
</tr>
<tr>
<td>1 f 6..1'</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 e 6..1'</td>
<td>2/3,1/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1 d 6..1'</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 c 6..1'</td>
<td>1/3,2/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b 6..1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a 6..1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1] p31'</th>
<th>Along [1,0,0] p1m11'</th>
<th>Along [2,1,0] p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^<em>=a \quad b^</em>=b )</td>
<td>( a^<em>=c \quad b^</em>=(a+2b)/2 )</td>
<td>( a^<em>=c \quad b^</em>/2 )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
**Hexagonal**


**Origin on \( \bar{6}' \)**

**Asymmetric unit**

\[
\begin{align*}
0 \leq x & \leq 2/3; & 0 \leq y & \leq 2/3; & 0 \leq z & \leq 1/2; & x & \leq (1+y)/2; & y & \leq \min(1-x,(1+x)/2) \\
\end{align*}
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2 & \quad 0,1/2,1/2 \\
\end{align*}
\]

**Symmetry Operations**

1. \( 1 \)
2. \( 3^* \quad 0,0,z \)
3. \( 3^* \quad 0,0,z \)
4. \( m' \quad x,y,0 \)
5. \( \bar{6}' \quad 0,0,z; 0,0,0 \)
6. \( \bar{6}''. \quad 0,0,z; 0,0,0 \)

\[
\begin{align*}
(1 | 0,0,0) & \quad (3_z | 0,0,0) & \quad (3_z^{-1} | 0,0,0) \\
(m_z | 0,0,0)' & \quad (\bar{6}_z | 0,0,0)' & \quad (6_z | 0,0,0)'
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 l 1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w] (4) x,y,z [u,v,w] (5) y,x-y,z [v,u-v,w] (6) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>3 k m'..</td>
<td>x,y,1/2 [u,v,0] y,x-y,1/2 [v,u-v,0] x+y,x,1/2 [u+v,u,0]</td>
</tr>
<tr>
<td>3 j m'..</td>
<td>x,y,0 [u,v,0] y,x-y,0 [v,u-v,0] x+y,x,0 [u+v,u,0]</td>
</tr>
<tr>
<td>2 i 3..</td>
<td>2/3,1/3,z [0,0,w] 2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>2 h 3..</td>
<td>1/3,2/3,z [0,0,w] 1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>2 g 3..</td>
<td>0,0,z [0,0,w] 0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1 f 6'..</td>
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</tr>
<tr>
<td>1 b 6'..</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a 6'..</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p3</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on $\overline{6}$

**Asymmetric unit**

- $0 \leq x \leq 2/3$;
- $0 \leq y \leq 2/3$;
- $0 \leq z \leq 1/2$;
- $x \leq (1+y)/2$;
- $y \leq \min(1-x,(1+x)/2)$

**Vertices**

- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/2$
- $1/2,0,1/2$
- $2/3,1/3,1/2$
- $1/3,2/3,1/2$
- $0,1/2,1/2$

**Symmetry Operations**

For $(0,0,0)$ + set

1. $1$
2. $3^+ 0,0,z$
3. $3^- 0,0,z$
4. $m x,y,0$
   - $(m_z|0,0,0)$
5. $\overline{2}^- 0,0,z; 0,0,0$
   - $(6_z^{-1}|0,0,0)$
6. $\overline{6}^+ 0,0,z; 0,0,0$
   - $(6_z|0,0,0)$

For $(0,0,1)$' + set

1. $t' (0,0,1)$
   - $(1|0,0,1)'$
2. $3' - (0,0,1) 0,0,z$
   - $(3_z|0,0,1)'$
3. $3' (0,0,1) 0,0,z$
   - $(3_z^{-1}|0,0,1)'$
4. $m' x,y,1/2$
   - $(m_z|0,0,1)'$
5. $\overline{6}' - 0,0,z; 0,0,1/2$
   - $(6_z^{-1}|0,0,1)'$
6. $\overline{6}' 0,0,z; 0,0,1/2$
   - $(6_z|0,0,1)'$
Generators selected:

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>6</td>
<td>k</td>
<td>x,y,1/2 [u,v,0]</td>
<td>(2) y,x-y,z [v-u,v,w]</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>x,y,0 [0,0,w]</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>i</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>(4) x+y,x,z [v-u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>(5) x+y,x,z [v-u,v,w]</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
<td>0,0,z [0,0,w]</td>
<td>(6) x+y,x,z [v-u,v,w]</td>
</tr>
<tr>
<td>2</td>
<td>f</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>2/3,1/3,0 [0,0,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>1/3,2/3,0 [0,0,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>0,0,1/2 [0,0,0]</td>
<td>(0,0,0) + (0,0,1)' +</td>
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<tr>
<td>2</td>
<td>a</td>
<td>0,0,0 [0,0,0]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31'    
Along [1,0,0] p2a 1m1     
Along [2,1,0] p2a 1m1

\[ a^* = a \quad b^* = b \]  
\[ a^* = c \quad b^* = (a + 2b)/2 \]  
\[ a^* = c \quad b^* = b/2 \]  

Origin at 0,0,z   
Origin at x,0,0    
Origin at x,x/2,0
Origin on center (6/m)

Asymmetric unit

\[
\begin{align*}
0 & \leq x \leq 2/3; \\
0 & \leq y \leq 1/2; \\
0 & \leq z \leq 1/2; \\
x & \leq (1+y)/2; \\
y & \leq \text{min}(1-x,x)
\end{align*}
\]

Vertices

\[
\begin{array}{cccc}
0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/2,1/2,0 \\
0,0,1/2 & 1/2,0,1/2 & 2/3,1/3,1/2 & 1/2,1/2,1/2
\end{array}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1,0,0,0) \\
(2) & \quad 3^+ \quad 0,0,z \\
(3) & \quad 3^+ \quad 0,0,z \\
(4) & \quad 2 \quad 0,0,z \\
(2_1) & \quad (0,0,0,0) \\
(5) & \quad 6^\cdot \quad 0,0,z \\
(6) & \quad 6^+ \quad 0,0,z \\
(7) & \quad \bar{1} \quad \bar{1},0,0,0 \\
(8) & \quad \bar{3}^+ \quad \bar{0},0,0,0 \\
(9) & \quad \bar{3}^+ \quad \bar{0},0,0,0 \\
(10) & \quad m \quad x,y,0 \\
(m_2) & \quad (0,0,0) \\
(11) & \quad 6^- \quad 0,0,z; \quad 0,0,0 \\
(12) & \quad 6^+ \quad 0,0,z; \quad 0,0,0
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

<table>
<thead>
<tr>
<th>Positions</th>
<th></th>
<th>Coordinates</th>
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<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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<td></td>
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<tr>
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<td>d</td>
<td>6..</td>
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<td>6/m..</td>
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<tr>
<td>1</td>
<td>a</td>
<td>6/m..</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p61'</th>
<th>Along [1,0,0]</th>
<th>p2'( m' )</th>
<th>Along [2,1,0]</th>
<th>p2'( m' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a )</td>
<td>( b^* = b )</td>
<td>( a^* = c )</td>
<td>( b^* = (a+2b)/2 )</td>
<td>( a^* = c )</td>
<td>( b^* = b/2 )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td>Origin at x,0,0</td>
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<td></td>
</tr>
</tbody>
</table>

175.1.1367 - 2 - 2972
Origin on center (6/m1')

Asymmetric unit

\[
\begin{align*}
0 & \leq x \leq 2/3; & 0 & \leq y \leq 1/2; & 0 & \leq z \leq 1/2; & x & \leq (1+y)/2; & y & \leq \min(1-x,x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/2,1/2,0 \\
0,0,1/2 & & 1/2,0,1/2 & & 2/3,1/3,1/2 & & 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & & (1) & & (1) & & (1) \\
1 & & 3^* & & 3 & & 3^* \\
(1|0,0,0) & & (0,0,z) & & (0,0,z) & & (0,0,z) \\
(3) & & (3) & & (3) & & (3)
\end{align*}
\]

\[
\begin{align*}
(2) & & (2) & & (2) & & (2) \\
2 & & 6^- & & 6^+ & & 6^+
\end{align*}
\]

\[
\begin{align*}
(4) & & (4) & & (4) \\
0,0,z & & 0,0,z & & 0,0,z \\
(2_z,0,0,0) & & (6_z,0,0,0) & & (6_z,0,0,0)
\end{align*}
\]

\[
\begin{align*}
(5) & & (5) & & (5) \\
6^- & & 6^- & & 6^- \\
(6_z,0,0,0) & & (6_z,0,0,0) & & (6_z,0,0,0)
\end{align*}
\]

\[
\begin{align*}
(7) & & (7) & & (7) \\
\overline{1} & & \overline{3}^* & & \overline{3}^* \\
(0,0,0) & & (0,0,0) & & (0,0,0)
\end{align*}
\]

\[
\begin{align*}
(8) & & (8) & & (8) \\
\overline{3}^* & & \overline{3}^* & & \overline{3}^*
\end{align*}
\]

\[
\begin{align*}
(9) & & (9) & & (9) \\
0,0,z; 0,0,0 & & 0,0,z; 0,0,0 & & 0,0,z; 0,0,0 \\
(3_z,0,0,0) & & (3_z,0,0,0) & & (3_z,0,0,0)
\end{align*}
\]

\[
\begin{align*}
(10) & & (10) & & (10) \\
m & & 6^- & & 6^- \\
(x,y,0) & & (0,0,z; 0,0,0) & & (0,0,z; 0,0,0) \\
(m_z,0,0,0) & & (6_z,0,0,0) & & (6_z,0,0,0)
\end{align*}
\]

\[
\begin{align*}
(11) & & (11) & & (11) \\
6^- & & 6^- & & 6^- \\
(0,0,z; 0,0,0) & & (0,0,z; 0,0,0) & & (0,0,z; 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(12) & & (12) \\
6^+ & & 6^+ & & 6^+
\end{align*}
\]

(6_z,0,0,0)
Continued

For 1' + set

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<table>
<thead>
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<tbody>
<tr>
<td>1'</td>
<td>3'</td>
<td>3'</td>
</tr>
<tr>
<td>(1) 1'</td>
<td>(2) 3'</td>
<td>(3) 3'</td>
</tr>
<tr>
<td>(1) 0,0,0'</td>
<td>(3) 0,0,0'</td>
<td>(3) 0,0,0'</td>
</tr>
<tr>
<td>(2) 0,0,0'</td>
<td>(6) 0,0,0'</td>
<td>(6) 0,0,0'</td>
</tr>
<tr>
<td>(7) 1'</td>
<td>(8) 3'</td>
<td>(9) 3'</td>
</tr>
<tr>
<td>(1) 0,0,0'</td>
<td>(3) 0,0,0'</td>
<td>(3) 0,0,0'</td>
</tr>
<tr>
<td>(2) 0,0,0'</td>
<td>(6) 0,0,0'</td>
<td>(6) 0,0,0'</td>
</tr>
<tr>
<td>(10) m'</td>
<td>(11) 6'</td>
<td>(12) 6'</td>
</tr>
<tr>
<td>(m) 0,0,0'</td>
<td>(6) 0,0,0'</td>
<td>(6) 0,0,0'</td>
</tr>
</tbody>
</table>

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>1 + 1' +</td>
<td></td>
</tr>
<tr>
<td>12 l 11'</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(4) x,y,z [0,0,0]</td>
<td>(5) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(7) x,y,z [0,0,0]</td>
<td>(8) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(10) x,y,z [0,0,0]</td>
<td>(11) x,y,z [0,0,0]</td>
</tr>
</tbody>
</table>

6 k m..1' x,y,1/2 [0,0,0] y,x,y,1/2 [0,0,0] x+y,x,1/2 [0,0,0]
|             |             |
| 6 j m..1'   |             |
| (x,y,0 [0,0,0] | (y,x,0 [0,0,0] | (x+y,x,0 [0,0,0] |
| (x,y,0 [0,0,0] | (y,x,0 [0,0,0] | (x+y,x,0 [0,0,0] |

6 i 2..1' 1/2,0,z [0,0,0] 0,1/2,z [0,0,0] 1/2,1/2,z [0,0,0]
|             |             |
| 4 h 3..1'   |             |
| (1/3,2/3,z [0,0,0] | (2/3,1/3,z [0,0,0] | (1/3,2/3,z [0,0,0] |

3 g 2/m..1' 1/2,0,1/2 [0,0,0] 0,1/2,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]

3 f 2/m..1' 1/2,0,0 [0,0,0] 0,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0]

2 e 6..1' 0,0,z [0,0,0] 0,0,z [0,0,0]

2 d 6..1' 1/3,2/3,1/2 [0,0,0] 2/3,1/3,1/2 [0,0,0]

2 c 6..1' 1/3,2/3,0 [0,0,0] 2/3,1/3,0 [0,0,0]

1 b 6/m..1' 0,0,1/2 [0,0,0]
1  a  6/m..1'  0,0,0 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
</table>
| [0,0,1]    | p61'       | a* = a  b* = b  
|            |            | Origin at 0,0,z |
| [1,0,0]    | p2mm1'     | a* = c  b* = (a + 2b)/2  
|            |            | Origin at x,0,0 |
| [2,1,0]    | p2mm1'     | a* = c  b* = b/2  
|            |            | Origin at x,x/2,0 |
**Origin** on center (6'/m)

**Asymmetric unit**

\[
0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x, x)
\]

**Vertices**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
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<tbody>
<tr>
<td>0,0,0</td>
<td>0,0,1/2</td>
<td>1/2,0,0</td>
<td>1/2,1/2</td>
<td>1/2,1/2,0</td>
</tr>
<tr>
<td>1/2,0,1/2</td>
<td>2/3,1/3,0</td>
<td>2/3,1/3,1/2</td>
<td>1/2,1/2,1/2</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry Operations**

\[
\begin{align*}
&\text{(1) } 1 \\
&(1 | 0,0,0) \\
&\text{(2) } 3^+ \quad 0,0,z \\
&(3z | 0,0,0) \\
&\text{(3) } 3^- \quad 0,0,z \\
&(3z^{-1} | 0,0,0) \\
&\text{(4) } 2' \quad 0,0,z \\
&(2z | 0,0,0)' \\
&\text{(5) } 6' \quad 0,0,z \\
&(6z^{-1} | 0,0,0)' \\
&\text{(6) } 6'' \quad 0,0,z \\
&(6z | 0,0,0)' \\
&\text{(7) } \overline{1}' \\
&(1 | 0,0,0)'' \\
&\text{(8) } 3' \quad 0,0,z; 0,0,0 \\
&(3z | 0,0,0)' \\
&\text{(9) } 3'' \quad 0,0,z; 0,0,0 \\
&(3z^{-1} | 0,0,0)' \\
&\text{(10) } m \quad x,y,0 \\
&(mz | 0,0,0) \\
&\text{(11) } 6^- \quad 0,0,z; 0,0,0 \\
&(6z^{-1} | 0,0,0) \\
&\text{(12) } 6^+ \quad 0,0,z; 0,0,0 \\
&(6z | 0,0,0)
\end{align*}
\]
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
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<tr>
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<td>a</td>
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**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p61'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
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<tr>
<td>Origin at 0,0,z</td>
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<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
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<tr>
<td>Origin at x,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
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</tbody>
</table>
**Origin** on center (6/m’)

**Asymmetric unit**

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x) \]

**Vertices**

- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/2,1/2,0
- 0,0,1/2
- 1/2,0,1/2
- 2/3,1/3,1/2
- 1/2,1/2,1/2

**Symmetry Operations**

1. \(1\)
   - \((1|0,0,0)\)
2. \(3^+\)
   - \((0,0,z)\)
   - \((3_z|0,0,0)\)
3. \(3^-\)
   - \((0,0,z)\)
   - \((3_z^{-1}|0,0,0)\)
4. \(2\)
   - \((0,0,z)\)
   - \((2_z|0,0,0)\)
5. \(6^+\)
   - \((0,0,z)\)
   - \((6_z|0,0,0)\)
6. \(6^-\)
   - \((0,0,z)\)
   - \((6_z^{-1}|0,0,0)\)
7. \(\bar{1}\)
   - \((1|0,0,0)^\prime\)
   - \((3_z^{-1}|0,0,0)^\prime\)
   - \((3_z|0,0,0)^\prime\)
8. \(3^+\)
   - \((0,0,z)\)
   - \((3_z|0,0,0)^\prime\)
   - \((3_z^{-1}|0,0,0)^\prime\)
9. \(3^-\)
   - \((0,0,z)\)
   - \((3_z|0,0,0)^\prime\)
   - \((3_z^{-1}|0,0,0)^\prime\)
10. \(m^-\)
    - \((x,y,0)\)
    - \((m_x|0,0,0)^\prime\)
11. \(6^+\)
    - \((0,0,z)\)
    - \((6_z|0,0,0)^\prime\)
12. \(6^-\)
    - \((0,0,z)\)
    - \((6_z^{-1}|0,0,0)^\prime\)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>12</td>
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<tr>
<td>6</td>
<td>k</td>
<td>m'..</td>
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<tr>
<td>6</td>
<td>j</td>
<td>m'..</td>
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<td>6</td>
<td>i</td>
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<td>4</td>
<td>h</td>
<td>3..</td>
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<tr>
<td>3</td>
<td>g</td>
<td>2/m'..</td>
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<td>3</td>
<td>f</td>
<td>2/m'..</td>
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<td>2</td>
<td>d</td>
<td>6'..</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>6'..</td>
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<tr>
<td>1</td>
<td>b</td>
<td>6/m'..</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>6/m'..</td>
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</table>

### Coordinates

<table>
<thead>
<tr>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) y,x-y,z [v,u-v,w]</th>
<th>(3) x+y,x,z [u+v,u,w]</th>
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<tbody>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y,x+y,z [v,u+v,w]</td>
<td>(6) x-y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td>(7) x,y,z [u,v,w]</td>
<td>(8) y,x+y,z [v,u+v,w]</td>
<td>(9) x-y,x,z [u-v,u,w]</td>
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<tr>
<td>(10) x,y,z [u,v,w]</td>
<td>(11) y,x-y,z [v,u-v,w]</td>
<td>(12) x+y,x,z [u+v,u,w]</td>
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<tr>
<td>(13) x,y,z [u,v,w]</td>
<td>(14) y,x-z [v,u+w]</td>
<td>(15) x,y,z [u,v,w]</td>
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<tr>
<td>(16) x,y,z [u,v,w]</td>
<td>(17) y,x-z [v,u+w]</td>
<td>(18) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

**Along [0,0,1]**

- p6'  
  - a = a  
  - b = b
  - Origin at 0,0,z

**Along [1,0,0]**

- p2m'm'  
  - a = c  
  - b = (a + 2b)/2  
  - a = c  
  - b = b/2  
  - Origin at x,0,0  
  - Origin at x,x/2,0

**Along [2,1,0]**

- p2m'm'  
  - a = c  
  - b = b/2  
  - Origin at x,x/2,0

---

175.4.1370 - 2 - 2979
**Origin** on center \((6'/m')\)

**Asymmetric unit**

\[
\begin{align*}
0 \leq x & \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x)
\end{align*}
\]

**Vertices**

\[
\begin{array}{cccc}
0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/2,1/2,0 \\
0,0,1/2 & 1/2,0,1/2 & 2/3,1/3,1/2 & 1/2,1/2,1/2 \\
\end{array}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 & (2) & \quad 3^{+} 0,0,z \\
\quad (1|0,0,0) & & (3) & \quad 3^{-} 0,0,z \\
\quad 0,0,0 & & (3_{z}|0,0,0) & \quad (3_{z}^{-1}|0,0,0) \\
(4) & \quad 2' 0,0,z & (5) & \quad 6' 0,0,z \\
\quad (2_{z}|0,0,0)' & & (6) & \quad 6^{+} 0,0,z \\
\quad (1|0,0,0) & & (6_{z}|0,0,0)' & \quad (6_{z}^{-1}|0,0,0)' \\
(7) & \quad \overline{1} 0,0,0 & (8) & \quad 3^{+} 0,0,z; 0,0,0 \\
\quad (1|0,0,0) & & (9) & \quad 3^{+} 0,0,z; 0,0,0 \\
\quad 0,0,0 & & (3_{z}|0,0,0) & \quad (3_{z}^{-1}|0,0,0) \\
(10) & \quad m' \ x,y,0 & (11) & \quad 6^{-} 0,0,z; 0,0,0 \\
\quad (m_{z}|0,0,0)' & & (12) & \quad 6^{+} 0,0,z; 0,0,0 \\
\quad x,y,0 & & (6_{z}|0,0,0)' & \quad (6_{z}^{-1}|0,0,0)' \\
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
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<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y,x+y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
<td>(8) y,x+y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) x,y,z [u,v,w]</td>
<td>(11) y,x-y,z [v,u-v,w]</td>
</tr>
</tbody>
</table>

| 6 k m'..     | x,y,1/2 [u,v,0] | y,x-y,1/2 [v,u-v,0] | x+y,x,1/2 [u+v,u,0] |
|              | x,y,1/2 [u,v,0] | y,x+y,1/2 [v,u-v,0] | x-y,x,1/2 [u+v,u,0] |

| 6 j m'..     | x,y,0 [u,v,0] | y,x-y,0 [v,u-v,0] | x+y,x,0 [u+v,u,0] |
|              | x,y,0 [u,v,0] | y,x+y,0 [v,u-v,0] | x-y,x,0 [u+v,u,0] |

| 6 i 2'..     | 1/2,0,z [u,v,0] | 0,1/2,z [v,u-v,0] | 1/2,1/2,z [u+v,u,0] |
|              | 1/2,0,z [u,v,0] | 0,1/2,z [v,u-v,0] | 1/2,1/2,z [u+v,u,0] |

| 4 h 3..      | 1/3,2/3,z [0,0,w] | 2/3,1/3,z [0,0,w] | 1/3,2/3,z [0,0,w] |
|              | 1/3,2/3,z [0,0,w] | 2/3,1/3,z [0,0,w] | 1/3,2/3,z [0,0,w] |

| 3 g 2'..     | 1/2,0,1/2 [u,v,0] | 0,1/2,1/2 [v,u-v,0] | 1/2,1/2,1/2 [u+v,u,0] |
|              | 1/2,0,1/2 [u,v,0] | 0,1/2,1/2 [v,u-v,0] | 1/2,1/2,1/2 [u+v,u,0] |

| 3 f 2'..     | 1/2,0,0 [u,v,0] | 0,1/2,0 [v,u-v,0] | 1/2,1/2,0 [u+v,u,0] |
|              | 1/2,0,0 [u,v,0] | 0,1/2,0 [v,u-v,0] | 1/2,1/2,0 [u+v,u,0] |

| 2 e 6'..     | 0,0,z [0,0,0] | 0,0,z [0,0,0] | 0,0,z [0,0,0] |
|              | 0,0,z [0,0,0] | 0,0,z [0,0,0] | 0,0,z [0,0,0] |

| 2 d 6'..     | 1/3,2/3,z [0,0,0] | 2/3,1/3,z [0,0,0] | 1/3,2/3,z [0,0,0] |
|              | 1/3,2/3,z [0,0,0] | 2/3,1/3,z [0,0,0] | 1/3,2/3,z [0,0,0] |

| 2 c 6'..     | 1/3,2/3,0 [0,0,0] | 2/3,1/3,0 [0,0,0] | 1/3,2/3,0 [0,0,0] |
|              | 1/3,2/3,0 [0,0,0] | 2/3,1/3,0 [0,0,0] | 1/3,2/3,0 [0,0,0] |

| 1 b 6'm'..   | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |
|              | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |

| 1 a 6'm'..   | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p6' Along [1,0,0] p2'2mm' Along [2,1,0] p2'2mm'

a* = a b* = b a* = (a + 2b)/2 b* = c a* = b/2 b* = c

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0

175.5.1371 - 2 - 2981
Origin on center (6/m)

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq 2/3; \\
0 \leq y & \leq 1/2; \\
0 \leq z & \leq 1/2; \\
x & \leq (1+y)/2; \\
y & \leq \text{min}(1-x, x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 \\
0,0,1/2 & \quad 1/2,0,1/2 \\
2/3,1/3,0 & \quad 2/3,1/3,1/2
\end{align*}
\]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1^* & \quad 0,0,z) \\
(2) & \quad 3^+ \quad 0,0,z \\
(3^* & \quad 0,0,z) \\
(3) & \quad 3 \quad 0,0,z \\
(3^* & \quad 0,0,z) \\
(4) & \quad 2 \quad 0,0,z \\
(2^* & \quad 0,0,z) \\
(5) & \quad 6^+ \quad 0,0,z \\
(6^* & \quad 0,0,z) \\
(6) & \quad 6 \quad 0,0,z \\
(6^* & \quad 0,0,z) \\
(7) & \quad m \quad x,y,0 \\
(7^* & \quad x,y,0) \\
(8) & \quad 3^+ \quad 0,0,z; 0,0,0 \\
(3^* & \quad 0,0,z; 0,0,0) \\
(9) & \quad 3^+ \quad 0,0,z; 0,0,0 \\
(3^* & \quad 0,0,z; 0,0,0) \\
(10) & \quad m \quad x,y,0 \\
(10^* & \quad x,y,0) \\
(11) & \quad 6^+ \quad 0,0,z; 0,0,0 \\
(6^* & \quad 0,0,z; 0,0,0) \\
(12) & \quad 6^+ \quad 0,0,z; 0,0,0 \\
(6^* & \quad 0,0,z; 0,0,0)
\end{align*}
\]
Continued 175.6.1372 P\_\_\_\_6/m

For (0,0,1)' + set

(1) t' (0,0,1)
(1) (0,0,1)'

(2) 3' t' (0,0,1) 0,0,z
(3) 3' t' (0,0,1) 0,0,z

(4) 2' (0,0,1) 0,0,z
(2) (0,0,1)'

(5) 6' (0,0,1) 0,0,z
(6) 6' (0,0,1) 0,0,z

(7) T' 0,0,1/2
(T | 0,0,1)'

(8) 3' 0,0,z; 0,0,1/2
(3 | 0,0,1)'

(10) m' x,y,1/2
(m | 0,0,1)'

(11) 6' 0,0,z; 0,0,1/2
(6 | 0,0,1)'

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
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<tr>
<td>12</td>
<td>k m’. x,y,1/2 [u,v,0] y,x-y,1/2 [v,u-v,0] x+y,x,1/2 [u+v,u,0]</td>
</tr>
<tr>
<td>12</td>
<td>j m.. x,y,0 [0,0,w] y,x-y,0 [0,0,w] x+y,x,0 [0,0,w]</td>
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<tr>
<td>12</td>
<td>i 2.. 1/2,0,z [0,0,w] 0,1/2,z [0,0,w] 1/2,1/2,z [0,0,w]</td>
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<tr>
<td>8</td>
<td>h 3.. 1/3,2/3,z [0,0,0] 1/3,2/3,z [0,0,w] 2/3,1/3,z [0,0,w] 1/3,2/3,z [0,0,w]</td>
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<td>6</td>
<td>g 2’/m’. 1/2,0,1/2 [u,v,0] 0,1/2,1/2 [v,u-v,0] 1/2,1/2,1/2 [u+v,u,0]</td>
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<tr>
<td>6</td>
<td>f 2/m.. 1/2,0,0 [0,0,w] 0,1/2,0 [0,0,w] 1/2,1/2,0 [0,0,w]</td>
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<td>4</td>
<td>d 6.. 1/3,2/3,1/2 [0,0,w] 2/3,1/3,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>c 6.. 1/3,2/3,0 [0,0,w] 2/3,1/3,0 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b 6/m’. 0,0,1/2 [0,0,0]</td>
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</tbody>
</table>
Continued

2  a  6/m..  0,0,0 [0,0,w]

**Symmetry of Special Projections**

Along [0,0,1]  p61'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)
Origin at 0,0,z

Along [1,0,0]  p_{2a'2m'm'}  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)
Origin at x,0,1/2

Along [2,1,0]  p_{2a'2m'm'}  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)
Origin at x,x/2,1/2
Origin on center (6'/m)

Asymmetric unit

\begin{align*}
0 \leq x & \leq 2/3; \\
0 \leq y & \leq 1/2; \\
0 \leq z & \leq 1/2; \\
x & \leq (1+y)/2; \\
y & \leq \min(1-x,x)
\end{align*}

Vertices

\begin{align*}
0,0,0 & \quad 1/2,0,0 \\
0,0,1/2 & \quad 1/2,0,1/2 \\
0,0,1/2 & \quad 1/2,0,1/2 \\
0,0,1/2 & \quad 1/2,0,1/2
\end{align*}

Symmetry Operations

For \((0,0,0) + \text{set} \)

\begin{align*}
(1) & \quad 1 \\
(10) & \quad m \ x,y,0 \\
(11) & \quad 6^+ \ 0,0,z; \ 0,0,0 \\
(12) & \quad 6^+ \ 0,0,z; \ 0,0,0
\end{align*}

\begin{align*}
(2) & \quad 3^+ \ 0,0,z \\
& \quad (3_z|0,0,0) \\
(5) & \quad 6^- \ 0,0,z \\
& \quad (6_z|0,0,0)' \\
(8) & \quad 3^+ \ 0,0,z; \ 0,0,0 \\
& \quad (3_z|0,0,0)''
\end{align*}

\begin{align*}
(3) & \quad 3^+ \ 0,0,z \\
& \quad (3_z|0,0,0) \\
(6) & \quad 6^+ \ 0,0,z \\
& \quad (6_z|0,0,0)'
\end{align*}

\begin{align*}
(4) & \quad 2' \ 0,0,z \\
& \quad (2_z|0,0,0)'
\end{align*}

\begin{align*}
(7) & \quad 3^+ \ 0,0,z \\
& \quad (3_z|0,0,0)''
\end{align*}

\begin{align*}
(9) & \quad 3^+ \ 0,0,z; \ 0,0,0 \\
& \quad (3_z|0,0,0)''
\end{align*}

\begin{align*}
(11) & \quad 6^- \ 0,0,z; \ 0,0,0 \\
& \quad (6_z|0,0,0)
\end{align*}
Generators selected

(1) $t'(0,0,1)$
(2) $3' (0,0,1)$ $0,0,z$
(3) $3' (0,0,1) 0,0,z$
(4) $2 (0,0,1) 0,0,z$
(5) $6^{-} (0,0,1) 0,0,z$
(6) $6^{-} (0,0,1) 0,0,z$
(7) $\overline{1} 0,0,1/2$
(8) $3^{-} 0,0,z; 0,0,1/2$
(9) $3^{-} 0,0,z; 0,0,1/2$
(10) $m' x,y,1/2$
(11) $6^{-'} 0,0,z; 0,0,1/2$
(12) $6^{-'} 0,0,z; 0,0,1/2$

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1) +</td>
<td>(0,0,0) + (0,0,1) +</td>
</tr>
</tbody>
</table>

Coordinates

For $(0,0,1)' + set$

(1) $t'(0,0,1)$
(2) $3' (0,0,1)$ $0,0,z$
(3) $3' (0,0,1) 0,0,z$
(4) $2 (0,0,1) 0,0,z$
(5) $6^{-} (0,0,1) 0,0,z$
(6) $6^{-} (0,0,1) 0,0,z$
(7) $\overline{1} 0,0,1/2$
(8) $3^{-} 0,0,z; 0,0,1/2$
(9) $3^{-} 0,0,z; 0,0,1/2$
(10) $m' x,y,1/2$
(11) $6^{-'} 0,0,z; 0,0,1/2$
(12) $6^{-'} 0,0,z; 0,0,1/2$

Generators selected

(1); $t(1,0,0); t(0,1,0); t'(0,0,1)$; (2); (4); (7).
Symmetry of Special Projections

Along [0,0,1] \( p61' \)
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] \( p2a^* \) 2mm
\[ a^* = c \quad b^* = (a + 2b)/2 \]
Origin at x,0,0

Along [2,1,0] \( p2a^* \) 2mm
\[ a^* = c \quad b^* = b/2 \]
Origin at x,x/2,0
Origin at center $\overline{3}$ on $6_3$

Asymmetric unit  
$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$

Vertices  
$0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0 \quad 0,0,1/4 \quad 1/2,0,1/4 \quad 2/3,1/3,1/4 \quad 1/3,2/3,1/4 \quad 0,1/2,1/4$

Symmetry Operations

(1) 1

(2) $3^+ \quad 0,0,z$

(3) $3^- \quad 0,0,z$

(4) $2 \quad (0,0,1/2) \quad 0,0,z$

(5) $6 \quad (0,0,1/2) \quad 0,0,z$

(6) $6^+ \quad (0,0,1/2) \quad 0,0,z$

(7) $\overline{1} \quad (1,0,0)$

(8) $\overline{3}^+ \quad 0,0,z; \quad 0,0,0$

(9) $\overline{3}^- \quad 0,0,z; \quad 0,0,0$

(10) $m \quad x,y,1/4$

(11) $6^- \quad 0,0,z; \quad 0,0,1/4$

(12) $6^+ \quad 0,0,z; \quad 0,0,1/4$
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions
Multiplicity, Wyckoff letter, Site Symmetry, Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 1</td>
<td>1</td>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
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<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
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<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
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<td>(5) y,x+y,z+1/2 [v,u+v,w]</td>
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<td>(6) x-y,x,z+1/2 [u-v,u,w]</td>
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<td>(7) x,y,z [u,v,w]</td>
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<td>(8) y,x+y,z [v,u-v,w]</td>
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<td>(9) x-y,x,z [u+v,u,w]</td>
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<td>(10) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(11) y,x-y,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(12) x+y,x,z+1/2 [u-v,u,w]</td>
</tr>
</tbody>
</table>

6 h m.. x,y,1/4 [0,0,w] y,x-y,1/4 [0,0,w] x+y,x,1/4 [0,0,w]
6 g t 1/2,0,0 [u,v,w] 0,1/2,0 [v,u-v,w] 1/2,1/2,0 [u+v,u,w]
1/2,0,1/2 [u,v,w] 0,1/2,1/2 [v,u+v,w] 1/2,1/2,1/2 [u-v,u,w]
4 f 3.. 1/3,2/3,z [0,0,w] 2/3,1/3,z+1/2 [0,0,w] 2/3,1/3,z [0,0,w] 1/3,2/3,z+1/2 [0,0,w]
4 e 3.. 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w] 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w]
2 d 6.. 2/3,1/3,1/4 [0,0,w] 1/3,2/3,3/4 [0,0,w]
2 c 6.. 1/3,2/3,1/4 [0,0,w] 2/3,1/3,3/4 [0,0,w]
2 b 3.. 0,0,0 [0,0,w] 0,0,1/2 [0,0,w]
2 a 6.. 0,0,1/4 [0,0,w] 0,0,3/4 [0,0,w]

Symmetry of Special Projections
Along [0,0,1] p6
a* = a b* = b
Origin at 0,0,z
Along [1,0,0] p2'mg'
a* = c b* = (a + 2b)/2
Origin at x,0,0
Along [2,1,0] p2'mg'
a* = c b* = b/2
Origin at x,x/2,0

Continued
Origin at center $\overline{3}1'$ on $6_31'$

Asymmetric unit

$$0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{4}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,(1+x)/2)$$

Vertices

$$0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0$$
$$0,0,1/4 \quad 1/2,0,1/4 \quad 2/3,1/3,1/4 \quad 1/3,2/3,1/4 \quad 0,1/2,1/4$$

Symmetry Operations

For 1 + set

1. $1$
   $$(1 | 0,0,0)$$

2. $3'$ $0,0,z$
   $$(3_{z} | 0,0,0)$$

3. $3'$ $0,0,z$
   $$(3_{z}^{-1} | 0,0,0)$$

4. $2$ $0,0,1/2$ $0,0,z$
   $$(2_{z} | 0,0,1/2)$$

5. $6$ $0,0,1/2$ $0,0,z$
   $$(6_{z}^{-1} | 0,0,1/2)$$

6. $6'$ $0,0,1/2$ $0,0,z$
   $$(6_{z} | 0,0,1/2)$$

7. $1$
   $$(1 | 0,0,0)$$

8. $3'$ $0,0,z; 0,0,0$
   $$(3_{z} | 0,0,0)$$

9. $3'$ $0,0,z; 0,0,0$
   $$(3_{z}^{-1} | 0,0,0)$$

10. $m$ $x,y,1/4$
    $$(m_{z} | 0,0,1/2)$$

11. $6$ $0,0,z; 0,0,1/4$
    $$(6_{z}^{-1} | 0,0,1/2)$$

12. $6'$ $0,0,z; 0,0,1/4$
    $$(6_{z} | 0,0,1/2)$$

$\text{P6}_3/m1'$

$6/m1'$

$\text{Hexagonal}$

176.2.1375 - 1 - 2990
Continued

176.2.1375 P6$_3$/m1'

For 1' + set

<table>
<thead>
<tr>
<th>(1) 1'</th>
<th>(2) 3'</th>
<th>(3) 3'</th>
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</thead>
<tbody>
<tr>
<td>1 (0,0,0)'</td>
<td>0,0,z</td>
<td>0,0,z</td>
</tr>
<tr>
<td>(3z</td>
<td>0,0,0)'</td>
<td>(3z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) 2' (0,0,1/2) 0,0,z</th>
<th>(5) 6' (0,0,1/2) 0,0,z</th>
<th>(6) 6' (0,0,1/2) 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2z</td>
<td>0,0,1/2)'</td>
<td>(6z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) 11'</th>
<th>(8) 3'</th>
<th>(9) 3'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(11</td>
<td>0,0,0)'</td>
<td>0,0,0</td>
</tr>
<tr>
<td>(3z</td>
<td>0,0,0)'</td>
<td>(3z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) m' x,y,1/4</th>
<th>(11) 6' 0,0,z; 0,0,1/4</th>
<th>(12) 6' 0,0,z; 0,0,1/4</th>
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</thead>
<tbody>
<tr>
<td>(mz</td>
<td>0,0,1/2)'</td>
<td>(6z</td>
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</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry.</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 + 1' +</td>
<td>1 + 1' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>12</th>
<th>i</th>
<th>11'</th>
<th>(1) x,y,z [0,0,0]</th>
<th>(2) y,x-y,z [0,0,0]</th>
<th>(3) x+y,x,z [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4)</td>
<td>x,y,z+1/2 [0,0,0]</td>
<td>(5) y,x+y,z+1/2 [0,0,0]</td>
<td>(6) x-y,x,z+1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7)</td>
<td>x,y,z [0,0,0]</td>
<td>(8) y,x+y,z [0,0,0]</td>
<td>(9) x-y,x,z [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(10)</td>
<td>x,y,z+1/2 [0,0,0]</td>
<td>(11) y,x-y,z+1/2 [0,0,0]</td>
<td>(12) x+y,x,z+1/2 [0,0,0]</td>
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<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>6</th>
<th>h</th>
<th>m..1'</th>
<th>x,y,1/4 [0,0,0]</th>
<th>y,x-y,1/4 [0,0,0]</th>
<th>x+y,x,1/4 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3)</td>
<td>x,y,3/4 [0,0,0]</td>
<td>y,x+y,3/4 [0,0,0]</td>
<td>x-y,x,3/4 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6</th>
<th>g</th>
<th>11'</th>
<th>1/2,0,0 [0,0,0]</th>
<th>0,1/2,0 [0,0,0]</th>
<th>1/2,1/2,0 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>f</th>
<th>3..1'</th>
<th>1/3,2/3,z [0,0,0]</th>
<th>2/3,1/3,z+1/2 [0,0,0]</th>
<th>2/3,1/3,z [0,0,0]</th>
<th>1/3,2/3,z+1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4)</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th>d</th>
<th>6..1'</th>
<th>2/3,1/3,1/4 [0,0,0]</th>
<th>1/3,2/3,3/4 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>c</td>
<td>6..1'</td>
<td>1/3,2/3,1/4 [0,0,0]</td>
<td>2/3,1/3,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>6..1'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>6..1'</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>
**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Direction</th>
<th>p61'</th>
<th>p2mg1'</th>
<th>p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>(a^* = a) (b^* = b)</td>
<td>(a^* = c) (b^* = (a + 2b)/2)</td>
<td>(a^* = c) (b^* = b/2)</td>
</tr>
<tr>
<td>Origin</td>
<td>0,0,z</td>
<td>x,0,0</td>
<td>x,x/2,0</td>
</tr>
</tbody>
</table>

Continued
**Origin** at center $\bar{3}'$ on $6_3'$

**Asymmetric unit**: $0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$

**Vertices**

- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,1/2,0$
- $0,0,1/4$
- $1/2,0,1/4$
- $2/3,1/3,1/4$
- $1/3,2/3,1/4$
- $0,1/2,1/4$

**Symmetry Operations**

1. $1$
2. $3^*$; $0,0,z$
3. $3'$; $0,0,z$
4. $2'$; $(0,0,1/2)$
5. $6'$; $(0,0,1/2)$
6. $6'$; $(0,0,1/2)$
7. $\bar{1}'$
8. $3''^*$; $0,0,0$
9. $\bar{3}''^*$; $0,0,0$
10. $m$; $x,y,1/4$
11. $6^*$; $0,0,1/4$
12. $6^*$; $0,0,1/4$
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>12</td>
<td>i</td>
<td>1 (1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<tr>
<td></td>
<td>1</td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
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<td>1</td>
<td>(5) y,x+y,z+1/2 [v,u-v,w]</td>
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<td>(12) x+y,x,z+1/2 [u-v,u,w]</td>
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<td>h</td>
<td>m.. x,y,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>y,x-y,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x+y,x,1/4 [0,0,w]</td>
</tr>
<tr>
<td>6</td>
<td>g</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
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<td>0,1/2,0 [0,0,0]</td>
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<td>1/2,1/2 [0,0,0]</td>
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<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>f</td>
<td>3.. 1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
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<td>1/3,2/3,z+1/2 [0,0,w]</td>
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<tr>
<td>4</td>
<td>e</td>
<td>3.. 0,0,z [0,0,w]</td>
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<td>0,0,z+1/2 [0,0,w]</td>
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<tr>
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<td>0,0,z [0,0,w]</td>
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<td>0,0,z+1/2 [0,0,w]</td>
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<td>d</td>
<td>6.. 2/3,1/3,1/4 [0,0,w]</td>
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<td></td>
<td></td>
<td>1/3,2/3,3/4 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>6.. 1/3,2/3,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,3/4 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>3.. 0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>6.. 0,0,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,3/4 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'                Along [1,0,0] p2mg                Along [2,1,0] p2mg
a* = a   b* = b                 a* = c   b* = (a + 2b)/2          a* = c   b* = b/2
Origin at 0,0,z                  Origin at x,0,0                  Origin at x,x/2,0
Origin at center $\bar{3}^+$ on $6_3$

Asymmetric unit

$$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)$$

Vertices

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3</td>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
</tr>
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<tr>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
<td>2/3,1/3,1/4</td>
<td>1/3,2/3,1/4</td>
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<td>1/2,0,1/4</td>
<td>2/3,1/3,1/4</td>
<td>1/3,2/3,1/4</td>
<td>0,1/2,1/4</td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) $1$

(1) $0,0,0$

(2) $3^+ 0,0,z$

(3) $3^- 0,0,z$

(4) $\bar{1} 2 (0,0,1/2) 0,0,z$

(5) $6^- (0,0,1/2) 0,0,z$

(6) $6^- (0,0,1/2) 0,0,z$

(7) $\bar{1} 0,0,0$

(8) $3^- 0,0,0$

(9) $3^- 0,0,0$

(10) $m' x,y,1/4$

(11) $6^- (0,0,1/4) (6^- z^- 0,0,1/2)$

(12) $6^- 0,0,z; 0,0,1/4$

$\bar{6}^- z^- 0,0,1/2$
Continued

176.4.1377

P6₃/m'

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

| 12 | i | 1 | (1) x,y,z [u,v,w] | (2) y,x-y,z [v,u-v,w] | (3) x+y,x-z [u+v,u,w] |
| (4) x,y,z+1/2 [u,v,w] | (5) y,x+y,z+1/2 [v,u+v,w] | (6) x-y,x+z+1/2 [u-v,u,w] |
| (7) x,y,z [u,v,w] | (8) y,x+y,z [v,u+v,w] | (9) x-y,x-z [u-v,u,w] |
| (10) x,y,z+1/2 [u,v,w] | (11) y,x-y,z+1/2 [v,u-v,w] | (12) x+y,x,z+1/2 [u+v,u,w] |

| 6 | h | m'.. | x,y,1/4 [u,v,0] | y,x-y,1/4 [v,u-v,0] | x+y,x,1/4 [u+v,u,0] |
| 6g | T | 1/2,0,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 1/2,0,1/2 [0,0,0] | 0,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

| 4 | f | 3.. | 1/3,2/3,z [0,0,w] | 2/3,1/3,z+1/2 [0,0,w] | 2/3,1/3,z [0,0,w] |
| 4 | e | 3.. | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z [0,0,w] |
| 0,0,z+1/2 [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z+1/2 [0,0,w] |

| 2 | d | 6.. | 2/3,1/3,1/4 [0,0,0] | 1/3,2/3,3/4 [0,0,0] |
| 2 | c | 6.. | 1/3,2/3,1/4 [0,0,0] | 2/3,1/3,3/4 [0,0,0] |

| 2 | b | 3.. | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] |
| 2 | a | 6.. | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p6

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

Along [1,0,0] p2m'g'

\[ a^* = c \quad b^* = (a + 2b)/2 \]

Origin at x,0,0

Along [2,1,0] p2m'g'

\[ a^* = c \quad b^* = b/2 \]

Origin at x,x/2,0
Origin at center $\bar{3}$ on $6_{3}'$

Asymmetric unit

\begin{align*}
0 \leq x \leq 2/3; & \quad 0 \leq y \leq 2/3; & \quad 0 \leq z \leq 1/4; & \quad x \leq (1+y)/2; & \quad y \leq \min(1-x,(1+x)/2) \\
0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/3,2/3,0 & 0,1/2,0 \\
0,0,1/4 & 1/2,0,1/4 & 2/3,1/3,1/4 & 1/3,2/3,1/4 & 0,1/2,1/4
\end{align*}

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(1) & \quad (0,0,0) \\
(2) & \quad 3^{+} 0,0,z \\
(3) & \quad 3^{-} 0,0,z \\
(4) & \quad 2' (0,0,1/2) 0,0,z \\
(5) & \quad 6' (0,0,1/2) 0,0,z \\
(6) & \quad 6' (0,0,1/2) 0,0,z \\
(7) & \quad \overline{1} \\
(8) & \quad \overline{3}^{-} 0,0,z; 0,0,0 \\
(9) & \quad \overline{3}^{+} 0,0,z; 0,0,0 \\
(10) & \quad m' x,y,1/4 \\
(11) & \quad 6^{-} 0,0,z; 0,0,1/4 \\
(12) & \quad 6^{+} 0,0,z; 0,0,1/4
\end{align*}

176.5.1378 - 1 - 2997
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>i</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>h</td>
<td>m'</td>
</tr>
<tr>
<td>6</td>
<td>g</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>f</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>6</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>6</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>6</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6'</th>
<th>Origin at 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2'm'g</th>
<th>Origin at x,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p2'm'g</th>
<th>Origin at x,x/2,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = b/2</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 622

Asymmetric unit: 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; x ≤ (1+y)/2; y ≤ min(1-x,x)

Vertices:
- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/2,1/2,0
- 0,0,1/2
- 1/2,0,1/2
- 2/3,1/3,1/2
- 1/2,1/2,1/2

Symmetry Operations:

1. 1
2. 3* 0,0,z
3. 3* 0,0,z
4. 2 0,0,z
5. 6* 0,0,z
6. 6* 0,0,z
7. 2 x,x,0
8. 2 x,0,0
9. 2 0,y,0
10. 2 x,x,0
11. 2 x,2x,0
12. 2 2x,x,0
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 n 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x-y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,x,y,z [u,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x+y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,y,z [u-u-v,w]</td>
</tr>
<tr>
<td>6 m .2 x,1/2 [u,u,0]</td>
<td>x,2x,1/2 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td>2x,x,1/2 [2u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>2x,x,1/2 [2u,u,0]</td>
</tr>
<tr>
<td>6 l .2 x,0 [u,u,0]</td>
<td>x,x,0 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td>2x,x,0 [2u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>2x,x,0 [2u,u,0]</td>
</tr>
<tr>
<td>6 k .2 x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>2x,x,1/2 [2u,u,0]</td>
</tr>
<tr>
<td>6 j .2 x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>6 i 2. 1/2,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>4 h 3. 1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>3 g 222 1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 f 222 1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>2 e 6. 0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d 3.2 1/3,2/3,1/2 [0,0,0]</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 3.2 1/3,2/3,0 [0,0,0]</td>
<td>2/3,1/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b 622 0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a 622 0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p6m'\text{'} \quad a^* = a \quad b^* = b

Along [1,0,0] p2m'\text{'} \quad a^* = c \quad b^* = \frac{(a + 2b)}{2}

Along [2,1,0] p2m'\text{'} \quad a^* = c \quad b^* = \frac{b}{2}

Origin at 0,0,z

Origin at x,0,0

Origin at x,x/2,0
**Origin** on 6221

**Asymmetric unit**

- $0 \leq x \leq 2/3;
- 0 \leq y \leq 1/2;
- 0 \leq z \leq 1/2;
- x \leq (1+y)/2;
- y \leq \min(1-x,x)$

**Vertices**

- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/2,1/2,0
- 0,0,1/2
- 1/2,0,1/2
- 2/3,1/3,1/2
- 1/2,1/2,1/2

**Symmetry Operations**

For 1 + set

1. $1$
2. $3^*$ 0,0,z
3. $3^{-1}$ 0,0,z
4. 0,0,z
5. $6^*$ 0,0,z
6. $6^{-1}$ 0,0,z
7. 0,0,0
8. x,x,0
9. x,0,0
10. x,x,0
11. x,2x,0
12. 2x,x,0
For 1' + set

(1) 1' (1,0,0)
       (1,0,0)
(2) 3' 0,0,0 (3) 3' 0,0,0
       (3,0,0)

(4) 2' 0,0,0 (5) 6' 0,0,0
       (6,0,0)
(2,0,0)
(6,0,0)

(7) 2' x,x,0 (8) 2' x,0,0
       (2,0,0)
(2,0,0)
(2,0,0)

(10) 2' x,x,0 (11) 2' x,2x,0
       (2,0,0)
(2,0,0)
(2,0,0)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>n, 11'</td>
<td>(1) x,y,z [0,0,0] (2) y,x,y,z [0,0,0] (3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>m, .21'</td>
<td>(4) x,y,z [0,0,0] (5) y,x+y,z [0,0,0] (6) x-y,x,z [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>l, .21'</td>
<td>(7) y,x,z [0,0,0] (8) x-y,x,y,z [0,0,0] (9) x,x+y,z [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>k, .21'</td>
<td>(10) y,x,z [0,0,0] (11) x+y,x,y,z [0,0,0] (12) x,x+y,z [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>j, .21'</td>
<td>(13) x,0,1/2 [0,0,0] (14) 0,x,1/2 [0,0,0] (15) x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>i, .21'</td>
<td>(16) x,0,0 [0,0,0] (17) 0,x,0 [0,0,0] (18) x,x,0 [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>h, .3.1'</td>
<td>(19) 1/2,0,z [0,0,0] (20) 0,1/2,z [0,0,0] (21) 1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>g, 2221'</td>
<td>(22) 1/2,0,1/2 [0,0,0] (23) 0,1/2,1/2 [0,0,0] (24) 1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>f, 2221'</td>
<td>(25) 1/2,0,0 [0,0,0] (26) 0,1/2,0 [0,0,0] (27) 1/2,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 +</td>
<td>1'</td>
<td>x,2x,1/2 [0,0,0] 2x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1'</td>
<td></td>
<td>x,x,1/2 [0,0,0] x,x,1/2 [0,0,0]</td>
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<tr>
<td>1'</td>
<td></td>
<td>x,x,0 [0,0,0] x,x,0 [0,0,0]</td>
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<tr>
<td>1'</td>
<td></td>
<td>x,x,1/2 [0,0,0] x,x,1/2 [0,0,0]</td>
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<tr>
<td>1'</td>
<td></td>
<td>0,x,0 [0,0,0] x,x,0 [0,0,0]</td>
</tr>
<tr>
<td>1'</td>
<td></td>
<td>0,1/2,0 [0,0,0] 1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>1'</td>
<td></td>
<td>1/3,2/3,z [0,0,0] 2/3,1/3,z [0,0,0] 1/3,2/3,z [0,0,0]</td>
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<tr>
<td>2</td>
<td>e</td>
<td>6..1'</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>3.21'</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>3.21'</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>6221'</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>6221'</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**  \( p6mm1' \)
  - \( a^* = a \)
  - \( b^* = b \)
  - Origin at 0,0,z

- **Along [1,0,0]**  \( p2mm1' \)
  - \( a^* = c \)
  - \( b^* = (a + 2b)/2 \)
  - Origin at x,0,0

- **Along [2,1,0]**  \( p2mm1' \)
  - \( a^* = c \)
  - \( b^* = b/2 \)
  - Origin at x,x/2,0
Origin on 6'2'2

Asymmetric unit

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 2/3;</td>
<td>0 ≤ y ≤ 1/2;</td>
<td>0 ≤ z ≤ 1/2;</td>
</tr>
<tr>
<td>x ≤ (1+y)/2;</td>
<td>y ≤ min(1-x,x)</td>
<td></td>
</tr>
</tbody>
</table>

Vertices

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
</tr>
<tr>
<td>0,0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1/3,1/2</td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) 1
(2) 3' 0,0,z
(3) 3' -1 0,0,z
(4) 2' 0,0,z
(5) 6' 0,0,z
(6) 6' -1 0,0,z
(7) 2' x,x,0
(8) 2' x,0,0
(9) 2' 0,y,0
(10) 2 x,x,0
(11) 2 x,2x,0
(12) 2 2x,x,0
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 n 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v-u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
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<td>(4) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z [v-u+v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x-y,x,z [u+v,u,w]</td>
</tr>
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<td></td>
<td>(7) y,x,z [v-u,w]</td>
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<td>(8) x-y,y,z [v-u-w]</td>
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</tr>
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<td>(10) y,x,z [v-u,w]</td>
</tr>
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<td>(11) x+y,y,z [u+u-w]</td>
</tr>
<tr>
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<td></td>
<td>(12) x-x-z [u-u+w]</td>
</tr>
<tr>
<td>6 m .2 x,</td>
<td>x,x,1/2 [u,u,0]</td>
<td>x,2x,1/2 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,1/2 [2u,0,0]</td>
</tr>
<tr>
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<td>x,2x,0 [u,2u,0]</td>
</tr>
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<td></td>
<td>2x,x,0 [2u,u,0]</td>
</tr>
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<td>6 k .2' x,</td>
<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
</tr>
<tr>
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<td>x,x,1/2 [u,u,w]</td>
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<td>6 j .2' x,</td>
<td>x,0,0 [u,2u,w]</td>
<td>0,x,0 [2u,u,w]</td>
</tr>
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<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td>6 i 2'.</td>
<td>1/2,0,0 [u,v,w]</td>
<td>0,1/2,0 [u,v,w]</td>
</tr>
<tr>
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<td></td>
<td>1/2,1/2,0 [2u,v,u]</td>
</tr>
<tr>
<td>4 h 3.</td>
<td>1/3,2,3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
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<td></td>
<td>1/3,2/3,z [0,0,w]</td>
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### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
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<tr>
<td>[0,0,1]</td>
<td>p6'm'm</td>
<td>0,0,z</td>
</tr>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
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</tr>
<tr>
<td>[1,0,0]</td>
<td>p2' mm'</td>
<td>x,0,0</td>
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<tr>
<td>a^* = (a + 2b)/2</td>
<td>b^* = c</td>
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<tr>
<td>[2,1,0]</td>
<td>p2mm</td>
<td>x,x/2,0</td>
</tr>
<tr>
<td>a^* = c</td>
<td>b^* = b/2</td>
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</table>
Origin on 6'22'

Asymmetric unit:
- $0 \leq x \leq 2/3$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$; $x \leq (1+y)/2$; $y \leq \min(1-x,x)$
- Vertices:
  - $(0,0,0)$
  - $(1/2,0,0)$
  - $(2/3,1/3,0)$
  - $(1/2,1/2,0)$
  - $(1/2,1/2,1/2)$

Symmetry Operations:

1. $1$
2. $3^*$ 0,0,z
3. $3^*$ 0,0,0

4. $2'$ 0,0,z
   \( (2_z,0,0) )^t \\
5. $6'$ 0,0,z
   \( (6_z^{-1},0,0) )^t \\
6. $6'$ 0,0,0

7. $2$ x,x,0
   \( (2_y,0,0) )^t \\
8. $2$ x,0,0
   \( (2_z,0,0) )^t \\
9. $2$ 0,y,0
   \( (2_y,0,0) )^t \\

10. $2'$ x,x,0
    \( (2_z,0,0) )^t \\
11. $2'$ x,2x,0
    \( (2_z,0,0) )^t \\
12. $2'$ 2x,x,0
    \( (2_z,0,0) )^t \\

177.4.1382 - 1 - 3008
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>12</td>
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<td>(1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w] (5) y,x+y,z [v,u-v,w] (6) x-y,x,z [u+v,u,w]</td>
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<tr>
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<td></td>
<td>(7) y,x,z [v,u,w] (8) x-y,y,z [v,u-v,w] (9) x,x+y,z [u,u+v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(10) y,x,z [v,u,w] (11) x+y,y,z [v,u-v,w] (12) x-y,x,z [u,u+v,w]</td>
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</table>

Coordinates

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
<tr>
<td>6 m</td>
<td>.2'</td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,2x,1/2 [u,0,w] 2x,x,1/2 [0,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,2x,1/2 [u,0,w] 2x,x,1/2 [0,u,w]</td>
</tr>
<tr>
<td>6 l</td>
<td>.2'</td>
<td>x,x,0 [u,u,w]</td>
<td>x,2x,0 [u,0,w] 2x,x,0 [0,u,w]</td>
</tr>
<tr>
<td></td>
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<td>x,x,0 [u,u,w]</td>
<td>x,2x,0 [u,0,w] 2x,x,0 [0,u,w]</td>
</tr>
<tr>
<td>6 k</td>
<td>.2</td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0] x,x,1/2 [u,u,0]</td>
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<tr>
<td></td>
<td></td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0] x,x,1/2 [u,u,0]</td>
</tr>
<tr>
<td>6 j</td>
<td>.2</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0] x,x,0 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0] x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>6 i</td>
<td>2'</td>
<td>1/2,0;z [u,v,0]</td>
<td>0,1/2,z [v,u-v,0] 1/2,1/2,z [u+v,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,z [v,u,0]</td>
<td>1/2,0;z [v,u-v,0] 1/2,1/2,z [u+v,u,0]</td>
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<tr>
<td>4 h</td>
<td>3</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w] 2/3,1/3,z [0,0,w]</td>
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<tr>
<td>3 g</td>
<td>22'</td>
<td>1/2,0,1/2 [u,0,0]</td>
<td>0,1/2,1/2 [0,u,0] 1/2,1/2,1/2 [u,u,0]</td>
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<tr>
<td>3 f</td>
<td>22'</td>
<td>1/2,0,0 [u,0,0]</td>
<td>0,1/2,0 [0,u,0] 1/2,1/2,0 [u,u,0]</td>
</tr>
<tr>
<td>2 e</td>
<td>6'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d</td>
<td>3'</td>
<td>1/3,2/3,1/2 [0,0,w]</td>
<td>2/3,1/3,1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 c</td>
<td>3'</td>
<td>1/3,2/3,0 [0,0,w]</td>
<td>2/3,1/3,0 [0,0,w]</td>
</tr>
<tr>
<td>1 b</td>
<td>6'22'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1 a</td>
<td>6'22'</td>
<td>0,0,0 [0,0,0]</td>
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</tr>
</tbody>
</table>
## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Case 1 (0,0,1) 06'mm'</th>
<th>Case 2 (1,0,0) p2mm</th>
<th>Case 3 (2,1,0) p2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Origin</strong></td>
<td>0,0,z</td>
<td>x,0,0</td>
<td>x,x/2,0</td>
</tr>
<tr>
<td><strong>Symmetry</strong></td>
<td><em><em>a</em> = a   b</em> = b**</td>
<td><em><em>a</em> = c   b</em> = (a + 2b)/2**</td>
<td><em><em>a</em> = b/2   b</em> = c**</td>
</tr>
</tbody>
</table>

Continued...
Origin on 62'2'

Asymmetric unit

\[
\begin{align*}
0 & \leq x \leq 2/3; & 0 & \leq y \leq 1/2; & 0 & \leq z \leq 1/2; & x & \leq (1+y)/2; & y & \leq \min(1-x,x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^{-1} \quad 0,0,z \\
(4) & \quad 2 \quad 0,0,z \\
(5) & \quad 6 \quad 0,0,z \\
(6) & \quad 6^{-1} \quad 0,0,z \\
(7) & \quad 2' \quad x,x,0 \\
(8) & \quad 2' \quad x,0,0 \\
(9) & \quad 2' \quad 0,y,0 \\
(10) & \quad 2' \quad x,x,0 \\
(11) & \quad 2' \quad x,0,0 \\
(12) & \quad 2' \quad 2x,0
\end{align*}
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

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<th>Coordinates</th>
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</tr>
</thead>
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<td>12 n 1</td>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y,x+y,z [v,u+v,w]</td>
<td>(6) x+y,x,z [u-v,u,w]</td>
<td>(7) y,x,z [v,u+w]</td>
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<tr>
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<td>(8) x+y,y,z [v,u+w]</td>
<td>(9) x+y,z [u+v,u,w]</td>
<td>(10) y,x,z [v,u+w]</td>
<td>(11) x+y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td>6 m .2'</td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,2x,1/2 [u,0,w]</td>
<td>2x,x,1/2 [0,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,x,1/2 [u,u,w]</td>
<td>x,2x,1/2 [u,0,w]</td>
<td>2x,x,1/2 [0,u,w]</td>
<td></td>
</tr>
<tr>
<td>6 l .2'</td>
<td>x,x,0 [u,u,w]</td>
<td>x,2x,0 [u,0,w]</td>
<td>2x,x,0 [0,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,x,0 [u,u,w]</td>
<td>x,2x,0 [u,0,w]</td>
<td>2x,x,0 [0,u,w]</td>
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</tr>
<tr>
<td>6 k .2'</td>
<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
<td>x,x,1/2 [u,u+w]</td>
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<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
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<tr>
<td>6 j .2'</td>
<td>x,0,0 [u,2u,w]</td>
<td>0,x,0 [2u,u,w]</td>
<td>x,x,0 [u,u+w]</td>
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<td>x,0,0 [u,2u,w]</td>
<td>0,x,0 [2u,u,w]</td>
<td>x,x,0 [u,u+w]</td>
<td></td>
</tr>
<tr>
<td>6 i 2.</td>
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<td>0,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
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<tr>
<td></td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
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</tr>
<tr>
<td>4 h 3.</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>1/3,2/3,z [0,0,w]</td>
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<tr>
<td>3 g 2'2'</td>
<td>1/2,0,1/2 [0,0,w]</td>
<td>0,1/2,1/2 [0,0,w]</td>
<td>1/2,1/2,1/2 [0,0,w]</td>
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<tr>
<td>3 f 2'2'</td>
<td>1/2,0,0 [0,0,w]</td>
<td>0,1/2,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
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</tr>
<tr>
<td>2 e 6.</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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</tr>
<tr>
<td>2 d 3.2'</td>
<td>1/3,2/3,1/2 [0,0,w]</td>
<td>2/3,1/3,1/2 [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>2 c 3.2'</td>
<td>1/3,2/3,0 [0,0,w]</td>
<td>2/3,1/3,0 [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>1 b 62'2'</td>
<td>0,0,1/2 [0,0,w]</td>
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<td></td>
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</tr>
<tr>
<td>1 a 62'2'</td>
<td>0,0,0 [0,0,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p6m' m'
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p2m' m'
\( a^* = c \quad b^* = (a + 2b)/2 \)
Origin at x,0,0

Along [2,1,0] p2'm' 'm'
\( a^* = c \quad b^* = b/2 \)
Origin at x,x/2,0
**Origin** on 622

**Asymmetric unit**

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x) \]

Vertices

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
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<tbody>
<tr>
<td>0,0</td>
<td>0,0</td>
<td>1/2</td>
</tr>
<tr>
<td>1/2,0,0</td>
<td>1/2,0,1/2</td>
<td>1/2,1/2,0</td>
</tr>
<tr>
<td>2/3,1/3,0</td>
<td>2/3,1/3,1/2</td>
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**Symmetry Operations**

For \((0,0,0) + \text{set}\)

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Symbol</th>
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<tr>
<td>(1)</td>
<td>(1</td>
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<tr>
<td>(2)</td>
<td>3*</td>
<td>0,0,z</td>
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<td>z</td>
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<td>(8)</td>
<td>(2</td>
<td>x</td>
</tr>
<tr>
<td>(9)</td>
<td>2</td>
<td>0,y,0</td>
</tr>
<tr>
<td>(9)</td>
<td>(2</td>
<td>y</td>
</tr>
<tr>
<td>(10)</td>
<td>2</td>
<td>x,x,0</td>
</tr>
<tr>
<td>(10)</td>
<td>(2</td>
<td>z</td>
</tr>
<tr>
<td>(11)</td>
<td>2</td>
<td>x,2x,0</td>
</tr>
<tr>
<td>(11)</td>
<td>(2</td>
<td>2x</td>
</tr>
<tr>
<td>(12)</td>
<td>2</td>
<td>2x,x,0</td>
</tr>
<tr>
<td>(12)</td>
<td>(2</td>
<td>2x</td>
</tr>
</tbody>
</table>
For $(0,0,1)' + \text{set}$

(1) $t'(0,0,1)$
   $(1'0,0,1)'$
(2) $3'(0,0,1)' 0,0,z$
   $(3_2'|0,0,1)'$
(3) $3'(0,0,1)' 0,0,z$
   $(3_2'|0,0,1)'$

(4) $2'(0,0,1) 0,0,z$
   $(2,0,0,0,0,0,0) 0,0,z$
(5) $6'(0,0,1) 0,0,z$
   $(6_2'|0,0,1)'$
(6) $6'(0,0,1) 0,0,z$
   $(6_2'|0,0,1)'$

(7) $2' x,x,1/2$
   $(2,0,0,0,0,0,0) x,x,1/2$
   $(2,0,0,0,0,0,0) x,x,1/2$
   $(2,0,0,0,0,0,0) x,x,1/2$
(8) $2' x,0,1/2$
   $(2,0,0,0,0,0,0) x,0,1/2$
   $(2,0,0,0,0,0,0) x,0,1/2$
   $(2,0,0,0,0,0,0) x,0,1/2$
(9) $2' 0,y,1/2$
   $(2,0,0,0,0,0,0) 0,y,1/2$
   $(2,0,0,0,0,0,0) 0,y,1/2$
   $(2,0,0,0,0,0,0) 0,y,1/2$

(10) $2' x,x,1/2$
    $(2,0,0,0,0,0,0) x,x,0$ [u,u,0]
    $(2,0,0,0,0,0,0) x,x,0$ [u,u,0]
    $(2,0,0,0,0,0,0) x,x,0$ [u,u,0]

Generators selected
(1); $t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7)$.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>12 m</th>
<th>x,x,1/2 [u,u,w]</th>
</tr>
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<tbody>
<tr>
<td>12 l</td>
<td>x,x,0 [u,u,0]</td>
</tr>
<tr>
<td>12 k</td>
<td>x,0,1/2 [u,2u,u]</td>
</tr>
<tr>
<td>12 j</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>12 i</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>8 h</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>6 g</td>
<td>2'2' 1/2,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>6 f</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
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</table>

Continued 177.6.1384 P 2_1 622

2/3,1/3,z [0,0,w] 2/3,1/3,z [0,0,w] 1/3,2/3,z [0,0,w] 1/2,1/2,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]
Continued

<table>
<thead>
<tr>
<th>4</th>
<th>e</th>
<th>6..</th>
<th>0,0,z [0,0,w]</th>
<th>0,0,z [0,0,w]</th>
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<tbody>
<tr>
<td>4</td>
<td>d</td>
<td>3.2'</td>
<td>1/3,2/3,1/2 [0,0,w]</td>
<td>2/3,1/3,1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>3.2</td>
<td>1/3,2/3,0 [0,0,0]</td>
<td>2/3,1/3,0 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>622</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>622</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
\[ a^* = a \quad b^* = b \]  
Origin at 0,0,z

Along [1,0,0] \( p_{2a^*}2m'm' \)  
\[ a^* = c \quad b^* = (a + 2b)/2 \]  
Origin at x,0,0

Along [2,1,0] \( p_{2a^*}2m'm' \)  
\[ a^* = c \quad b^* = b/2 \]  
Origin at x,x/2,0
Origin on 6'22'

Asymmetric unit

\[ 0 \leq x < \frac{2}{3}; \quad 0 \leq y < \frac{1}{2}; \quad 0 \leq z < \frac{1}{2}; \quad x < \frac{(1+y)}{2}; \quad y \leq \min(1-x, x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1') & \quad (1|0,0,0) \\
(2) & \quad 3^* \quad 0,0,z \\
(2') & \quad (3_z|0,0,0) \\
(3) & \quad 3^* \quad 0,0,z \\
(3') & \quad (3_z|0,0,0) \\
(4) & \quad 2' \quad 0,0,z \\
(4') & \quad (2_z|0,0,0) \\
(5) & \quad 6' \quad 0,0,z \\
(5') & \quad (6_z|0,0,0) \\
(6) & \quad 6^* \quad 0,0,z \\
(6') & \quad (6_z|0,0,0) \\
(7) & \quad 2 \quad x,x,0 \\
(7') & \quad (2_x|0,0,0) \\
(8) & \quad 2 \quad x,0,0 \\
(8') & \quad (2_x|0,0,0) \\
(9) & \quad 2 \quad 0,y,0 \\
(9') & \quad (2_y|0,0,0) \\
(10) & \quad 2' \quad x,x,0 \\
(10') & \quad (2_z|0,0,0) \\
(11) & \quad 2' \quad x,2x,0 \\
(11') & \quad (2_z|0,0,0) \\
(12) & \quad 2' \quad 2x,x,0 \\
(12') & \quad (2_z|0,0,0)
\end{align*}
\]
Continued

For $(0,0,1)' + \text{set}$

1. \( t'(0,0,1) \)
2. \( 3' \cdot (0,0,1) \) \( 0,0,z \)
3. \( 3' \cdot (0,0,1) \) \( 0,0,z \)

4. \( 2(0,0,1) \) \( 0,0,z \)
5. \( 6' \cdot (0,0,1) \) \( 0,0,z \)
6. \( 6' \cdot (0,0,1) \) \( 0,0,z \)

7. \( 2' \cdot x,x,1/2 \)
8. \( 2' \cdot x,0,1/2 \)
9. \( 2' \cdot 0,y,1/2 \)

10. \( 2 \cdot x,x,1/2 \)
11. \( 2 \cdot x,2x,1/2 \)
12. \( 2 \cdot 2x,x,1/2 \)

Generators selected \((1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).\)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>24 n 1</td>
<td>((0,0,0) + (0,0,1)' + )</td>
</tr>
<tr>
<td>(1) ( x,y,z [u,v,w])</td>
<td>(2) ( \bar{y},x-y,z [\bar{v},u-v,w])</td>
</tr>
<tr>
<td>(4) ( \bar{x},\bar{y},z [u,v,w])</td>
<td>(5) ( y,\bar{x}+y,z [\bar{v},u-v,\bar{w}])</td>
</tr>
<tr>
<td>(7) ( y,x,\bar{z} [v,u,\bar{w}])</td>
<td>(8) ( x-y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>(10) ( \bar{y},\bar{x},\bar{z} [v,u,w])</td>
<td>(11) ( \bar{x}+y,\bar{y},\bar{z} [u-v,\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>12 m .2</td>
<td>(x,\bar{x},1/2 [u,\bar{u},0])</td>
</tr>
<tr>
<td>(\bar{x},\bar{x},1/2 [u,\bar{u},0])</td>
<td>(\bar{x},2\bar{x},1/2 [u,2u,0])</td>
</tr>
<tr>
<td>12 l .2'</td>
<td>(x,\bar{x},0 [u,\bar{u},u])</td>
</tr>
<tr>
<td>(\bar{x},\bar{x},0 [u,\bar{u},w])</td>
<td>(\bar{x},2\bar{x},0 [u,0,\bar{w}])</td>
</tr>
<tr>
<td>12 k .2'.</td>
<td>(x,0,1/2 [u,2u,\bar{w}])</td>
</tr>
<tr>
<td>(\bar{x},0,1/2 [u,2u,\bar{w}])</td>
<td>(0,\bar{x},1/2 [2\bar{u},\bar{u},\bar{w}])</td>
</tr>
<tr>
<td>12 j .2.</td>
<td>(x,0,0 [u,0,0])</td>
</tr>
<tr>
<td>(\bar{x},0,0 [u,0,0])</td>
<td>(0,\bar{x},0 [0,u,0])</td>
</tr>
<tr>
<td>12 i .2'.</td>
<td>(1/2,0,0 [u,\bar{u},\bar{w}])</td>
</tr>
<tr>
<td>(0,1/2,\bar{z} [v,u,\bar{w}])</td>
<td>(1/2,0,\bar{z} [u-v,\bar{v},0])</td>
</tr>
<tr>
<td>8 h 3.</td>
<td>(1/3,2/3,\bar{z} [0,0,0])</td>
</tr>
<tr>
<td>6 g 22'</td>
<td>(1/2,0,1/2 [u,2u,0])</td>
</tr>
<tr>
<td>6 f 22'</td>
<td>(1/2,0,0 [u,0,0])</td>
</tr>
</tbody>
</table>

177.7.1385 - 2 - 3018
Symmetry of Special Projections

Along [0,0,1] \( p6mm' \)
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] \( p_{2a} \cdot 2mm \)
\( a^* = c \quad b^* = (a + 2b)/2 \)
Origin at x,0,0

Along [2,1,0] \( p_{2a} \cdot 2mm \)
\( a^* = c \quad b^* = b/2 \)
Origin at x,x/2,1/2

4 e 6'.. 0,0,z [0,0,0] 0,0,z [0,0,0]
4 d 3.2 1/3,2/3,1/2 [0,0,0] 2/3,1/3,1/2 [0,0,0]
4 c 3.2' 1/3,2/3,0 [0,0,w] 2/3,1/3,0 [0,0,w]
2 b 6'22' 0,0,1/2 [0,0,0] 0,0,0 [0,0,0]
2 a 6'22' 0,0,0 [0,0,0]
**Origin** on 2 [100] at 6, (2,1,1) 1

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/12 \]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 & \quad 0,1,0 \\
0,0,1/12 & \quad 1,0,1/12 & \quad 1,1,1/12 & \quad 0,1,1/12
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(1\ | 0,0,0) & \quad (2) & \quad 3^* (0,0,1/3) \quad 0,0,z \\
& \quad (3_z | 0,0,1/3) \quad (3) & \quad 3^* (0,0,2/3) \quad 0,0,z \\
& \quad (3_z | 0,0,2/3) \\
(4) & \quad 2 (0,0,1/2) \quad 0,0,z \\
(2_z | 0,0,1/2) & \quad (5) & \quad 6^* (0,0,5/6) \quad 0,0,z \\
& \quad (6_z | 0,0,5/6) \quad (6) & \quad 6^* (0,0,1/6) \quad 0,0,z \\
& \quad (6_z | 0,0,1/6) \\
(7) & \quad 2 x,x,1/6 \\
(2_{xy} | 0,0,1/3) & \quad (8) & \quad 2 x,0,0 \\
& \quad (2_z | 0,0,0) \quad (9) & \quad 2 0,y,1/3 \\
& \quad (2_y | 0,0,2/3) \\
(10) & \quad 2 x,x,5/12 \\
(2_z | 0,0,5/6) & \quad (11) & \quad 2 x,2x,1/4 \\
& \quad (2_{xy} | 0,0,1/2) \quad (12) & \quad 2 2x,x,1/12 \\
& \quad (2_z | 0,0,1/6)
\end{align*}
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 c 1 (1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z+1/3 [v,u-v,w]</td>
</tr>
<tr>
<td>(4) x,y,z+1/2 [u,v,w]</td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td>(7) y,x,z+1/3 [v,u,w]</td>
<td>(6) x-y,x,z+1/6 [u-v,u,w]</td>
</tr>
<tr>
<td>(10) y,x,z+5/6 [v,u,w]</td>
<td>(9) x,x+y,z+2/3 [u,u+v,w]</td>
</tr>
<tr>
<td>6 b .2 x,2x,1/4 [u,2u,0]</td>
<td>2x,x,7/12 [2u,u,0]</td>
</tr>
<tr>
<td>x,2x,3/4 [u,2u,0]</td>
<td>x,x,11/12 [u,u,0]</td>
</tr>
<tr>
<td>6 a .2 x,0,0 [u,0,0]</td>
<td>0,x,1/3 [0,u,0]</td>
</tr>
<tr>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,5/6 [0,u,0]</td>
</tr>
<tr>
<td>x,1/6 [u,u,0]</td>
<td>x,x,1/6 [u,u,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p6mm  
Along [1,0,0] p2m'g'  
Along [2,1,0] p2mg

\[a^* = a \quad b^* = b\]  
\[a^* = c \quad b^* = (a + 2b)/2\]  
\[a^* = c \quad b^* = b/2\]

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x/2,1/12
Origin on 21' [100] at 6, (2,1,1) 11'

Asymmetric unit

\[
\begin{align*}
0 \leq & x \leq 1; \\
0 \leq & y \leq 1; \\
0 \leq & z \leq 1/12
\end{align*}
\]

Vertices

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
</tr>
<tr>
<td>0,0,1/12</td>
<td>1,0,1/12</td>
<td>1,1,1/12</td>
</tr>
</tbody>
</table>

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) \ 1 & \quad (1) \ 1 \\
(1)0,0,0 & \quad (1)0,0,0 \\
(4) \ 2 & \quad (4) \ 2 \\
(0,0,1/2) \quad (0,0,1/2) & \quad (0,0,1/2) \\
(2z) \quad (2z) & \quad (2z) \\
(7) \ 2 & \quad (7) \ 2 \\
\ x,1/6 & \quad \ x,1/6 \\
(2x) & \quad (2x) \\
(2x,0,0,1/3) & \quad (2x,0,0,1/3) \\
(10) \ 2 & \quad (10) \ 2 \\
\ x,5/12 & \quad \ x,5/12 \\
(2x) & \quad (2x) \\
(2x,0,0,5/6) & \quad (2x,0,0,5/6) \\
(11) \ 2 & \quad (11) \ 2 \\
\ x,2x,1/4 & \quad \ x,2x,1/4 \\
(2x) & \quad (2x) \\
(2x,0,0,1/2) & \quad (2x,0,0,1/2) \\
(12) \ 2 & \quad (12) \ 2 \\
\ 2x,1/12 & \quad \ 2x,1/12 \\
(2x) & \quad (2x) \\
(2x,0,0,1/6) & \quad (2x,0,0,1/6)
\end{align*}
\]
For $1'$ + set

(1) $1'$  

(2) $3'$ $(0,0,1/3) 0,0,z$  

(3) $3'$ $(0,0,2/3) 0,0,z$  

(4) $2'$ $(0,0,1/2) 0,0,z$  

(5) $6'$ $(0,0,5/6) 0,0,z$  

(6) $6'$ $(0,0,1/6) 0,0,z$  

(7) $2'$ $\bar{x},x,1/6$  

(8) $2'$ $\bar{x},0,0$  

(9) $2'$ $0,y,1/3$  

(10) $2'$ $x,\bar{x},5/12$  

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1'$ + $1'$</td>
<td>$1'$</td>
</tr>
<tr>
<td>$2'$</td>
<td>$\bar{y},y,z+1/3 [0,0,0]$</td>
</tr>
<tr>
<td>$4'$</td>
<td>$y,x+y,z+5/6 [0,0,0]$</td>
</tr>
<tr>
<td>$7'$</td>
<td>$x-y,y,z [0,0,0]$</td>
</tr>
<tr>
<td>$X'$</td>
<td>$\bar{x}+y,y,\bar{z}+1/2 [0,0,0]$</td>
</tr>
<tr>
<td>$6'$</td>
<td>$x,2x,1/4 [0,0,0]$</td>
</tr>
<tr>
<td>$6'$</td>
<td>$\bar{x},2\bar{x},3/4 [0,0,0]$</td>
</tr>
<tr>
<td>$6'$</td>
<td>$x,0,0 [0,0,0]$</td>
</tr>
<tr>
<td>$6'$</td>
<td>$\bar{x},0,1/2 [0,0,0]$</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Along</th>
<th>Along</th>
<th>Along</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along $[0,0,1]$ p6mm1'</td>
<td>$a^* = a$, $b^* = b$</td>
<td>$a^* = c$, $b^* = (a + 2b)/2$</td>
<td>$a^* = c$, $b^* = b/2$</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x/2,1/12</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on 2' [100] at 6', (2',1,1) 1

**Asymmetric unit**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 1;</td>
<td>0 ≤ y ≤ 1;</td>
<td>0 ≤ z ≤ 1/12</td>
</tr>
</tbody>
</table>

**Vertices**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
</tr>
<tr>
<td>0,0,1/12</td>
<td>1,0,1/12</td>
<td>1,1,1/12</td>
</tr>
<tr>
<td></td>
<td>0,1,0</td>
<td>0,1,1/12</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

<table>
<thead>
<tr>
<th>Operation</th>
<th>(x,y,z)</th>
<th>(x,y,z)</th>
<th>(x,y,z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>(1 0 0)</td>
<td>(1 0 0)</td>
<td>(1 0 0)</td>
</tr>
<tr>
<td>(1 0 0)</td>
<td>(1 0 0)</td>
<td>(1 0 0)</td>
<td>(1 0 0)</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>(0,0,1/3)</td>
<td>(0,0,1/3)</td>
<td>(0,0,1/3)</td>
</tr>
<tr>
<td>(0,0,1/3)</td>
<td>(0,0,1/3)</td>
<td>(0,0,1/3)</td>
<td>(0,0,1/3)</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>(0,0,2/3)</td>
<td>(0,0,2/3)</td>
<td>(0,0,2/3)</td>
</tr>
<tr>
<td>(0,0,2/3)</td>
<td>(0,0,2/3)</td>
<td>(0,0,2/3)</td>
<td>(0,0,2/3)</td>
</tr>
<tr>
<td>(4) 2'</td>
<td>(0,0,1/2)</td>
<td>(0,0,1/2)</td>
<td>(0,0,1/2)</td>
</tr>
<tr>
<td>(0,0,1/2)</td>
<td>(0,0,1/2)</td>
<td>(0,0,1/2)</td>
<td>(0,0,1/2)</td>
</tr>
<tr>
<td>(5) 6'</td>
<td>(0,0,5/6)</td>
<td>(0,0,5/6)</td>
<td>(0,0,5/6)</td>
</tr>
<tr>
<td>(0,0,5/6)</td>
<td>(0,0,5/6)</td>
<td>(0,0,5/6)</td>
<td>(0,0,5/6)</td>
</tr>
<tr>
<td>(6) 6'</td>
<td>(0,0,1/6)</td>
<td>(0,0,1/6)</td>
<td>(0,0,1/6)</td>
</tr>
<tr>
<td>(0,0,1/6)</td>
<td>(0,0,1/6)</td>
<td>(0,0,1/6)</td>
<td>(0,0,1/6)</td>
</tr>
<tr>
<td>(7) 2'</td>
<td>(x,0)</td>
<td>(x,0)</td>
<td>(x,0)</td>
</tr>
<tr>
<td>(x,0)</td>
<td>(x,0)</td>
<td>(x,0)</td>
<td>(x,0)</td>
</tr>
<tr>
<td>(2) 2'</td>
<td>x,0</td>
<td>x,0</td>
<td>x,0</td>
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<td>x,0</td>
<td>x,0</td>
<td>x,0</td>
<td>x,0</td>
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<tr>
<td>(8) 2'</td>
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<tr>
<td>(x,0)</td>
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<td>(x,0)</td>
<td>(x,0)</td>
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<tr>
<td>(9) 2'</td>
<td>0,1/3</td>
<td>0,1/3</td>
<td>0,1/3</td>
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<td>0,1/3</td>
<td>0,1/3</td>
</tr>
<tr>
<td>(10) 2'</td>
<td>x,5/12</td>
<td>x,5/12</td>
<td>x,5/12</td>
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<td>x,5/12</td>
<td>x,5/12</td>
<td>x,5/12</td>
<td>x,5/12</td>
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<tr>
<td>(11) 2'</td>
<td>x,2x,1/4</td>
<td>x,2x,1/4</td>
<td>x,2x,1/4</td>
</tr>
<tr>
<td>x,2x,1/4</td>
<td>x,2x,1/4</td>
<td>x,2x,1/4</td>
<td>x,2x,1/4</td>
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<tr>
<td>(12) 2'</td>
<td>2x,1/12</td>
<td>2x,1/12</td>
<td>2x,1/12</td>
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<tr>
<td>2x,1/12</td>
<td>2x,1/12</td>
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</table>
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>12</td>
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<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z+1/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z+5/6 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x-y,x,z+1/6 [u+v,u,w]</td>
</tr>
<tr>
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<td></td>
<td>(7) y,x,z+1/3 [v,u,w]</td>
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<td></td>
<td>(8) x-y,y,z [u+v,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(9) x+y,z+2/3 [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y,x,z+5/6 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(11) x+y,y,z+1/2 [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) x,y,z+1/6 [u,u-v,w]</td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td>x,2x,1/4 [u,2u,0]</td>
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<tr>
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<td>2x,x,7/12 [2u,u,0]</td>
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<tr>
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<td></td>
<td>x,x,11/12 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,3/4 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,x,1/12 [2u,u,0]</td>
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<tr>
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<td>x,x,5/12 [u,u,0]</td>
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<tr>
<td>6</td>
<td>a</td>
<td>x,0,0 [u,2u,w]</td>
</tr>
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<td>0,x,1/3 [2u,u,0]</td>
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<tr>
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<td>x,x,2/3 [u,u,w]</td>
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<td>x,0,1/2 [u,2u,w]</td>
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<td>0,x,5/6 [2u,u,0]</td>
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<tr>
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<td>x,x,1/6 [u,u,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'mm'  Along [1,0,0] p2'm'g  Along [2,1,0] p2mg
\( a^* = a \)  \( b^* = b \)  \( a^* = c \)  \( b^* = (a + 2b)/2 \)  \( a^* = c \)  \( b^* = b/2 \)
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,1/12
**Origin** on 2 [100] at 6,' (2,1,1) 1

**Asymmetric unit**

\[
0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/12
\]

Vertices

- 0,0,0
- 0,0,1/12
- 1,0,0
- 1,0,1/12
- 1,1,0
- 1,1,1/12
- 0,1,0
- 0,1,1/12

**Symmetry Operations**

1. 1
   \( (1 | 0,0,0) \)

2. \( 3' (0,0,1/3) \) 0,0,z
   \( (3_z | 0,0,1/3) \)

3. \( 3' (0,0,2/3) \) 0,0,z
   \( (3_z^- | 0,0,2/3) \)

4. \( 2' (0,0,1/2) \) 0,0,z
   \( (2_z | 0,0,1/2) \)

5. \( 6' (0,0,5/6) \) 0,0,z
   \( (6_z^- | 0,0,5/6) \)

6. \( 6' (0,0,1/6) \) 0,0,z
   \( (6_z | 0,0,1/6) \)

7. \( 2 \times x,x,1/6 \)
   \( (2_{xy} | 0,0,1/3) \)

8. \( 2 \times x,0,0 \)
   \( (2_x | 0,0,0) \)

9. \( 2 \times 0,0,1/3 \)
   \( (2_z | 0,0,2/3) \)

10. \( 2' \times x,x,5/12 \)
    \( (2_z | 0,0,5/6) \)

11. \( 2' \times 2x,1/4 \)
    \( (2_{xy} | 0,0,1/2) \)

12. \( 2' \times 2x,1/12 \)
    \( (2_{xy} | 0,0,1/6) \)
Continued 178.4.1389  P6,'2' 22'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>c 1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z+1/3 [v,u-v,w] (3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w] (5) y,x+y,z+5/6 [v,u-v,w] (6) x-y,x,z+1/6 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x,z+1/3 [v,u,w] (8) x-y,y,z [u-v,v,w] (9) x,x+y,z+2/3 [u,u+v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y,x,z+5/6 [v,u,w] (11) x+y,y,z+1/2 [u-v,v,w] (12) x,x-y,z+1/6 [u,u+v,w]</td>
</tr>
<tr>
<td>6</td>
<td>b 2'</td>
<td>x,2x,1/4 [u,0,w] 2x,x,7/12 [0,u,w] x,x,11/12 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,3/4 [u,0,w] 2x,x,1/12 [0,u,w] x,x,5/12 [u,u,w]</td>
</tr>
<tr>
<td>6</td>
<td>a .2</td>
<td>x,0,0 [u,0,0] 0,x,1/3 [0,u,0] x,x,2/3 [u,u,0]</td>
</tr>
<tr>
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<td>x,0,1/2 [u,0,0] 0,x,5/6 [0,u,0] x,x,1/6 [u,u,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'km'  Along [1,0,0] p2mg  Along [2,1,0] p2mm'
a* = a  b* = b  a* = c  b* = (a + 2b)/2  a* = c  b* = b/2
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,1/12
**Origin** on \(2' [100] \) at \((2',1,1)\) 1

**Asymmetric unit**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 1;</td>
<td>0 ≤ y ≤ 1;</td>
<td>0 ≤ z ≤ 1/12</td>
</tr>
</tbody>
</table>

**Vertices**

<p>| | | |</p>
<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
</tr>
<tr>
<td>0,0,1/12</td>
<td>1,0,1/12</td>
<td>1,1,1/12</td>
</tr>
<tr>
<td>0,0,1/12</td>
<td>1,0,1/12</td>
<td>0,1,1/12</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. \(1\)
   \((1|0,0,0)\)
2. \(3^* (0,0,1/3) 0,0,z\)
   \((3_z,0,0,1/3)\)
3. \(3^* (0,0,2/3) 0,0,z\)
   \((3_z,0,0,2/3)\)
4. \(2 (0,0,1/2) 0,0,z\)
   \((2_z,0,0,1/2)\)
5. \(6^* (0,0,5/6) 0,0,z\)
   \((6_z,0,0,5/6)\)
6. \(6^* (0,0,1/6) 0,0,z\)
   \((6_z,0,0,1/6)\)
7. \(2' x,x,1/6\)
   \((2_{xy},0,0,1/3)'\)
8. \(2' x,0,0\)
   \((2_z,0,0,0)'\)
9. \(2' 0,y,1/3\)
   \((2_y,0,0,2/3)'\)
10. \(2' x,x,5/12\)
    \((2_{xy},0,0,5/6)'\)
11. \(2' x,2x,1/4\)
    \((2_z,0,0,1/2)'\)
12. \(2' 2x,x,1/12\)
    \((2_{1},0,0,1/6)'\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
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<tr>
<th>Multiplicity</th>
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<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>12 c 1 (1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z+1/3 [v,u-v,w]</td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td>(4) x,y,z+1/2 [u,v,w]</td>
<td>(5) y,x+y,z+5/6 [v,u+v,w]</td>
<td>(6) x-y,x,z+1/6 [u-v,u,w]</td>
</tr>
<tr>
<td>(7) y,x,z+1/3 [v,u,w]</td>
<td>(8) x-y,x-z [u+v,v,w]</td>
<td>(9) x+y,z+2/3 [u,u-v,w]</td>
</tr>
<tr>
<td>(10) y,x,z+5/6 [v,u,w]</td>
<td>(11) x+y,y,z+1/2 [u-v,v,w]</td>
<td>(12) x-y,x,z+1/6 [u+u+v,w]</td>
</tr>
</tbody>
</table>

6 b .2' x,2x,1/4 [u,0,w] 2x,x,7/12 [0,u,w] x,x,11/12 [u,u,w]
| 2x,x,1/12 [0,u,w] | x,x,5/12 [u,u,w] |

6 a .2': x,0,0 [u,2u,w] 0,x,1/3 [2u,u,w] x,x,2/3 [u,u,w]
| x,0,1/2 [u,2u,w] | 0,x,5/6 [2u,u,w] | x,x,1/6 [u,u,w] |

Symmetry of Special Projections

Along [0,0,1] p6mm Along [1,0,0] p2'mg' Along [2,1,0] p2'mg'

\[ a^* = a \quad b^* = b \]

\[ a^* = c \quad b^* = (a + 2b)/2 \]

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,1/12
Origin on 2 [100] at 65 (2,1,1) 1

Asymmetric unit

0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/12

Vertices

0,0,0 1,0,0 1,1,0 0,1,0
0,0,1/12 1,0,1/12 1,1,1/12 0,1,1/12

Symmetry Operations

(1) 1
(1 0,0,0)

(2) 3z (0,0,2/3) 0,0,z
(3z 0,0,2/3)

(3) 3z (0,0,1/3) 0,0,z
(3z 0,0,1/3)

(4) 2 (0,0,1/2) 0,0,z
(2z 0,0,1/2)

(5) 6z (0,0,1/6) 0,0,z
(6z 0,0,1/6)

(6) 6z (0,0,5/6) 0,0,z
(6z 0,0,5/6)

(7) 2 x,x,1/3
(2x 0,0,2/3)

(8) 2 x,0,0
(2 0,0,0)

(9) 2 0,y,1/6
(2y 0,0,1/3)

(10) 2 x,x,1/12
(2x 0,0,1/6)

(11) 2 x,2x,1/4
(2x 0,0,1/2)

(12) 2 2x,x,5/12
(2 0,0,5/6)
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

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<td>(10) y,x,z+1/6 [v,u,v]</td>
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<td>6 b .2</td>
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<td>x,2x,3/4 [u,2u,0]</td>
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<td>6 a .2</td>
<td></td>
<td>x,0,0 [u,0,0]</td>
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<tr>
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<td>x,0,1/2 [u,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6m'm' Along [1,0,0] p2m'g' Along [2,1,0] p2m'g'
a* = a b* = b a* = c b* = (a + 2b)/2 a* = c b* = b/2
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,5/12
Origin on 21' [100] at 6_3 (2,1,1) 11'

Asymmetric unit

\[
\begin{align*}
0 & \leq x \leq 1; & 0 & \leq y \leq 1; & 0 & \leq z \leq \frac{1}{12}
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1,0,0 & & 1,1,0 & & 0,1,0 \\
0,0,\frac{1}{12} & & 1,0,\frac{1}{12} & & 1,1,\frac{1}{12} & & 0,1,\frac{1}{12}
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & 1 & (2) & 3' (0,0,2/3) & 0,0,z \\
(1) & 1 & (3) & 3' (0,0,1/3) & 0,0,z \\
(4) & 2 (0,0,1/2) & 0,0,z & (3z) & 0,0,2/3 \\
(2z) & 0,0,1/2 & & (3z) & 0,0,1/3 \\
(7) & 2 & x,x,1/3 & (5) & 6' (0,0,1/6) & 0,0,z \\
(2xy) & 0,0,2/3 & & (6z) & 0,0,1/6 & & (6z) & 0,0,5/6 \\
(10) & 2 & x,x,1/12 & (8) & 2 & x,0,0 \\
(2z) & 0,0,1/6 & & (2z) & 0,0,0 & & (2z) & 0,0,1/3 \\
(11) & 2 & x,2x,1/4 & (9) & 2 & 0,y,1/6 \\
(2z) & 0,0,1/2 & & (2z) & 0,0,0 & & (2z) & 0,0,1/3 \\
(12) & 2 & 2x,x,5/12 & & (2z) & 0,0,5/6 \\
\end{align*}
\]
For 1' + set

(1) 1' (2) 3' (0,0,2/3) 0,0,z (3) 3' (0,0,1/3) 0,0,z
(1;0,0,0)' (3;0,0,2/3)' (3;0,0,1/3)'

(4) 2' (0,0,1/2) 0,0,z (5) 6' (0,0,1/6) 0,0,z
(2;0,0,1/2)' (6;0,0,1/6)'

(7) 2' x,x,1/3 (8) 2' x,0,0
(2;0,0,2/3)' (8;0,0,0)'

(10) 2' x,x,1/12 (11) 2' x,2x,1/4
(2;0,0,1/6)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 c 11'</td>
<td>x,y,z [0,0,0]</td>
<td>1' + x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,z+1/2 [0,0,0]</td>
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</tr>
<tr>
<td></td>
<td>y,x,y,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>y,x,z+2/3 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,y,y,z [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>y,x,z+1/6 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x+y,y,z+1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>6 b .21'</td>
<td>x,2x,3/4 [0,0,0]</td>
<td>1' + x,2x,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,2x,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,x,5/12 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>6 a .21'</td>
<td>x,0,0 [0,0,0]</td>
<td>1' + x,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x,x,5/6 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6mm1' Along [1,0,0] p2mg1' Along [2,1,0] p2mg1'
\[a^* = a \quad b^* = b\] \[a^* = c \quad b^* = (a + 2b)/2\] \[a^* = c \quad b^* = b/2\]
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,5/12
**Origin** on 2' [100] at 6s 1' (2',1,1) 1

**Asymmetric unit**

\[
\begin{align*}
0 & \leq x \leq 1; & 0 & \leq y \leq 1; & 0 & \leq z \leq \frac{1}{12} \\
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1,0,0 & & 1,1,0 & & 0,1,0 \\
0,0,\frac{1}{12} & & 1,0,\frac{1}{12} & & 1,1,\frac{1}{12} & & 0,1,\frac{1}{12} \\
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 & & (2) & \quad 3' (0,0,2/3) & \quad 0,0,z & & (3) & \quad 3' (0,0,1/3) & \quad 0,0,z \\
& \quad (1,0,0) & & (3,0,0,2/3) & & (3,0,0,1/3) & & (3,0,0,1/3) \\
(4) & \quad 2' (0,0,1/2) & \quad 0,0,z & & (5) & \quad 6' (0,0,1/6) & \quad 0,0,z & & (6) & \quad 6' (0,0,5/6) & \quad 0,0,z \\
& \quad (2,0,0,1/2)' & & (6,0,1/6)' & & (6,0,5/6)' & & (6,0,5/6)' \\
(7) & \quad 2' x,x,1/3 & \quad (2,0,0,1/3)' & & (8) & \quad 2' x,0,0 & \quad (2,0,0,0)' & & (9) & \quad 2' 0,y,1/6 & \quad (2,0,0,1/3)' \\
& \quad (2,0,2/3)' & & (2,0,0,0)' & & (2,0,0,0)' & & (2,0,0,1/3)' \\
(10) & \quad 2 x,x,1/12 & \quad (2,0,0,1/6) & & (11) & \quad 2 x,2x,1/4 & \quad (2,0,0,1/2) & & (12) & \quad 2x,5/12 & \quad (2,0,0,5/6) \\
& \quad (2,0,0,1/6) & & (2,0,0,1/2) & & (2,0,0,5/6) & & (2,0,0,5/6) \\
\end{align*}
\]
### Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z+1/6 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z+5/6 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+2/3 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x-y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x+y,z+1/3 [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/6 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x+y,y,z+1/2 [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,x-y,z+5/6 [u,u-v,w]</td>
</tr>
</tbody>
</table>

| 6 b 0.2                                      | x,2x,3/4 [u,2u,0] |
|                                             | 2x,x,5/12 [2u,u,0] |
|                                             | x,x,1/12 [u,u,0] |
|                                             | x,2x,1/4 [u,2u,0] |
|                                             | 2x,x,11/12 [2u,u,0] |
|                                             | x,x,7/12 [u,u,0] |

| 6 a 0.2'                                     | x,0,0 [u,2u,w] |
|                                             | 0,x,2/3 [2u,u,w] |
|                                             | x,x,1/3 [u,u,w] |
|                                             | x,0,1/2 [u,2u,w] |
|                                             | 0,x,1/6 [2u,u,w] |
|                                             | x,x,5/6 [u,u,w] |

### Symmetry of Special Projections

- **Along [0,0,1]**: p6'nm'
  - $a^* = a$, $b^* = b$
  - Origin at 0,0,z

- **Along [1,0,0]**: p2'm'g
  - $a^* = c$, $b^* = (a + 2b)/2$
  - Origin at x,0,0

- **Along [2,1,0]**: p2mg
  - $a^* = c$, $b^* = b/2$
  - Origin at x,x/2,5/12
Origin on 2 [100] at 65' (2,1,1) 1

Asymmetric unit
0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/12

Vertices
0,0,0 1,0,0 1,1,0 0,1,0
0,0,1/12 1,0,1/12 1,1,1/12 0,1,1/12

Symmetry Operations

1. 1
   (1 | 0,0,0)

2. 3' (0,0,2/3) 0,0,z
   (3z | 0,0,2/3)

3. 3' (0,0,1/3) 0,0,z
   (3z' | 0,0,1/3)

4. 2' (0,0,1/2) 0,0,z
   (2z | 0,0,1/2)

5. 6' (0,0,1/6) 0,0,z
   (6z | 0,0,1/6)

6. 6' (0,0,5/6) 0,0,z
   (6z' | 0,0,5/6)

7. 2 x,x,1/3
   (2xy | 0,0,2/3)

8. 2 x,0,0
   (2z | 0,0,0)

9. 2 0,y,1/6
   (2y | 0,0,1/3)

10. 2 x,x,1/12
    (2z | 0,0,1/6)

11. 2 x,2x,1/4
    (2z | 0,0,1/2)

12. 2 x,x,5/12
    (2z | 0,0,5/6)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 c 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z+1/6 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z+5/6 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x, x-z+2/3 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) y,y-z [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,x+yz+1/3 [u,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/6 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) y+y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x-x,y,z+5/6 [u,u+v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6'm'm</th>
<th>Along [1,0,0]</th>
<th>p2mg</th>
<th>Along [2,1,0]</th>
<th>p2'm'g</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a, b* = b</td>
<td>a* = c, b* = (a+2b)/2</td>
<td>a* = c, b* = b/2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,5/12</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Origin** on 2' [100] at 6₆ (2',1,1) 1

**Asymmetric unit**

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0 ≤ x ≤ 1;</th>
<th>0 ≤ y ≤ 1;</th>
<th>0 ≤ z ≤ 1/12</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
<td>0,1,0</td>
</tr>
<tr>
<td>0,0,1/12</td>
<td>1,0,1/12</td>
<td>1,1,1/12</td>
<td>0,1,1/12</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. (1) 1
   - (1) 0,0,0

2. (2) 3' (0,0,2/3) 0,0,z
   - (3) 3' (0,0,1/3) 0,0,z
   - (3') 0,0,1/3

3. (4) 2 (0,0,1/2) 0,0,z
   - (2) 0,0,1/2

4. (5) 6' (0,0,1/6) 0,0,z
   - (6') 0,0,5/6
   - (6') 0,0,1/6

5. (7) 2' x,x,1/3
   - (2') 0,0,2/3

6. (8) 2' x,0,0
   - (2') 0,0,0

7. (9) 2' y,0,1/6
   - (2') 0,0,1/3

8. (10) 2' x,x,1/12
   - (2') 0,0,1/6

9. (11) 2' x,2x,1/4
   - (2') 0,0,1/2

10. (12) 2' 2x,x,5/12
    - (2') 0,0,5/6

**P6₅2'2'**

**Hexagonal**

179.5.1395

**179.5.1395 - 1 - 3038**
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z+1/6 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z+5/6 [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+2/3 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x-y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x+y,x,z+1/3 [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/6 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x+y,y,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,x-y,z+5/6 [u,u+v,w]</td>
</tr>
</tbody>
</table>

| 6            | b .2' | x,2x,3/4 [u,0,w] |
|              |      | 2x,x,5/12 [0,u,w] |
|              |      | x,x,1/12 [u,u,w] |
| 6            | a .2' | x,0,0 [u,2u,w] |
|              |      | 0,x,2/3 [2u,0,w] |
|              |      | x,x,1/3 [u,u,w] |
|              |      | x,0,1/2 [u,2u,w] |
|              |      | 0,x,1/6 [2u,u,w] |
|              |      | x,x,5/6 [u,u,w] |

Symmetry of Special Projections

Along [0,0,1] p6mm
\( a^* = a \) \( b^* = b \)
Origin at 0,0,z

Along [1,0,0] p2'mg'
\( a^* = c \) \( b^* = (a + 2b)/2 \)
Origin at 0,0,0

Along [2,1,0] p2'mg'
\( a^* = c \) \( b^* = b/2 \)
Origin at x,0,0
Origin at 222 at 6\_2 (2,1,1) (1,2,1)

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \quad y \leq x \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 \\
0,0,1/6 & \quad 1,0,1/6 & \quad 1,1,1/6
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1\times0,0,0) \\
(2) & \quad 3' (0,0,2/3) \quad 0,0,z \\
& \quad (3_z\times0,0,2/3) \\
(3) & \quad 3' (0,0,1/3) \quad 0,0,z \\
& \quad (3_z\times0,0,1/3) \\
(4) & \quad 2 \quad 0,0,z \\
& \quad (2_z\times0,0,0) \\
(5) & \quad 6' (0,0,2/3) \quad 0,0,z \\
& \quad (6_z\times0,0,2/3) \\
(6) & \quad 6' (0,0,1/3) \quad 0,0,z \\
& \quad (6_z\times0,0,1/3) \\
(7) & \quad 2 \quad x,x,1/3 \\
& \quad (2_{xy}\times0,0,2/3) \\
(8) & \quad 2 \quad x,0,0 \\
& \quad (2_x\times0,0,0) \\
(9) & \quad 2 \quad 0,y,1/6 \\
& \quad (2_y\times0,0,1/3) \\
(10) & \quad 2 \quad x,\&1/3 \\
& \quad (2_z\times0,0,2/3) \\
(11) & \quad 2 \quad x,2x,0 \\
& \quad (2_{xy}\times0,0,0) \\
(12) & \quad 2 \quad 2x,x,1/6 \\
& \quad (2_{xy}\times0,0,1/3)
\end{align*}
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

## Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>k</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z+2/3 [v,u-v,w] (3) x+y,x,z+1/3 [u+v,u,w] (4) x,y,z [u,v,w] (5) x+y,z+2/3 [v,u+v,w] (6) x-y,x,z+1/3 [u-v,u,w] (7) x,x+y,z [u+v,v,w] (8) x-y,x,z+2/3 [u-v,u,w] (9) x,x+y,z+1/3 [u,u+v,w] (10) x,x,x+2/3 [u,u+2v,w] (11) x,x,y,z [u,v+w,w] (12) x,x,x+2/3 [u,u+2v,w]</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>(2) x,x,1/2 [u,2u,0] (3) x,x,1/2 [2u,u,0] (4) x,x,1/2 [u,v,w]</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>(5) x,x,3/2 [2u,u,0] (6) x,x,3/2 [u,v,w]</td>
</tr>
<tr>
<td>6</td>
<td>h</td>
<td>(7) x,1/2 [u,0,0] (8) x,1/2 [0,0,0] (9) x,1/2 [u,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>g</td>
<td>(10) x,1/2 [u,0,0] (11) x,1/2 [0,0,0] (12) x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>f</td>
<td>(13) x,1/2 [0,0,0] (14) x,1/2 [0,0,0] (15) x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>d</td>
<td>(16) x,1/2 [0,0,0] (17) x,1/2 [0,0,0] (18) x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>(19) x,1/2 [0,0,0] (20) x,1/2 [0,0,0] (21) x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>(22) x,1/2 [0,0,0] (23) x,1/2 [0,0,0] (24) x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>(25) x,1/2 [0,0,0] (26) x,1/2 [0,0,0] (27) x,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a</td>
<td>b' = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = c</td>
<td>b' = (a + 2b)/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = c</td>
<td>b' = b/2</td>
</tr>
<tr>
<td>Origin at x,x/2,1/6</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at 2221' at 6_2 (2,1,1) (1,2,1)1'

**Asymmetric unit**

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \quad y \leq x \]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 \\
0,0,1/6 & \quad 1,0,1/6 & \quad 1,1,1/6
\end{align*}
\]

**Symmetry Operations**

For 1 + set

1. \(1 \ (1^*,0,0,0)\)
2. \(3^* (0,0,2/3) 0,0,z\)
3. \(3^* (0,0,1/3) 0,0,z\)
4. \(2 0,0,z (2_z^*,0,0,0)\)
5. \(6 (0,2/3) 0,0,z (6_z^*0,0,2/3)\)
6. \(6^+ (0,1/3) 0,0,z (6_z^*0,0,1/3)\)
7. \(2 \ x,x,1/3 (2_{xy}^*,0,0,2/3)\)
8. \(2 \ x,0,0 (2_x^*0,0,0)\)
9. \(2 \ 0,y,1/6 (2_y^*0,0,1/3)\)
10. \(2 \ x,\&,1/3 (2_{3}^*,0,0,2/3)\)
11. \(2 \ x,2x,0 (2_x^*0,0,0)\)
12. \(2 \ 2x,x,1/6 (2_y^*0,0,1/3)\)

For 1' + set

1. \(1' \ (1^*,0,0,0)'\)
2. \(3' (0,0,2/3) 0,0,z\)
3. \(3' (0,0,1/3) 0,0,z\)
4. \(2' 0,0,z (2_{z}^*,0,0,0)\)
5. \(6' (0,2/3) 0,0,z (6_z^*0,0,2/3)\)
6. \(6' (0,1/3) 0,0,z (6_z^*0,0,1/3)\)
7. \(2' \ x,x,1/3 (2_{xy}^*,0,0,2/3)\)
8. \(2' \ x,0,0 (2_x^*0,0,0)\)
9. \(2' \ 0,y,1/6 (2_y^*0,0,1/3)\)
10. \(2' \ x,\&,1/3 (2_{3}^*,0,0,2/3)\)
11. \(2' \ x,2x,0 (2_x^*0,0,0)\)
12. \(2' \ 2x,x,1/6 (2_y^*0,0,1/3)\)
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>k 11'</td>
<td></td>
</tr>
</tbody>
</table>

### Coordinates

<table>
<thead>
<tr>
<th>1 +</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) y,x-y,z+2/3 [0,0,0]</td>
</tr>
<tr>
<td>(3) x+y,x,z+1/3 [0,0,0]</td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(5) y,x+y,z+2/3 [0,0,0]</td>
<td>(6) x-y,x,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td>(7) y,x,z+2/3 [0,0,0]</td>
<td>(8) x-y,y,z+2/3 [0,0,0]</td>
</tr>
<tr>
<td>(9) x,x+y,z+1/3 [0,0,0]</td>
<td>(10) y,x,z+2/3 [0,0,0]</td>
</tr>
<tr>
<td>(11) x+y,y,z+2/3 [0,0,0]</td>
<td>(12) x,y-z+1/3 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- Along [0,0,1] p6mm1'
  - $a^* = a$  
  - $b^* = b$
  - Origin at 0,0,z

- Along [1,0,0] p2mm1'
  - $a^* = c$  
  - $b^* = (a + 2b)/2$
  - Origin at x,0,0

- Along [2,1,0] p2mm1'
  - $a^* = c$  
  - $b^* = b/2$
  - Origin at x,x/2,1/6
### Origin
At 2'2'2' at $6_3^+$ (2',1,1) (1,2',1)

### Asymmetric unit

<table>
<thead>
<tr>
<th></th>
<th>0 ≤ x ≤ 1;</th>
<th>0 ≤ y ≤ 1;</th>
<th>0 ≤ z ≤ 1/6</th>
<th>y ≤ x</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices</td>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry Operations

1. 1
   - $1^{h0,0,0}$
2. $3^*$ (0,0,2/3) 0,0,z
   - $3_z^{*0,0,2/3}$
3. $3^*$ (0,0,1/3) 0,0,z
   - $3_z^{*0,0,1/3}$
4. $2'$ 0,0,z
   - $(2_z^{*0,0,0})'$
5. $6'$ (0,0,2/3) 0,0,z
   - $(6_z^{*0,0,2/3})'$
6. $6'$ (0,0,1/3) 0,0,z
   - $(6_z^{*0,0,1/3})'$
7. $2'$ x,x,1/3
   - $(2_{xy}^{*0,0,2/3})'$
8. $2'$ x,0,0
   - $(2_x^{*0,0,0})'$
9. $2'$ 0,y,1/6
   - $(2_y^{*0,0,1/3})'$
10. $2'$ x,y,1/3
    - $(2_z^{*0,0,2/3})$
11. $2'$ 0,x,2/3
    - $(2_{xy}^{*0,0,0})$
12. $2'$ 2x,x,1/6
    - $(2_z^{*0,0,1/3})$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 k 1</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x',y',z',2/3 [v',u',w']</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x',y',z' [u,v,w]</td>
<td>(5) y',x'+y',z'+2/3 [v',u-v,w']</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) x',y',z'+2/3 [v',u',w']</td>
<td>(8) y',x'+y',z'+u',v',w'</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y',x'+z'+2/3 [v',u',w']</td>
<td>(11) x'+y',y',z'+ [u'+v',u',w']</td>
</tr>
</tbody>
</table>

6 j .2 x,2x,1/2 [u,2u,0] 2x,2x,1/6 [2u,u,0] x,x,5/6 [u,u,0]

6 i .2 x,2x,0 [u,2u,0] 2x,2x,2/3 [2u,u,0] x,x,1/3 [u,u,0]

6 h .2' x,0,1/2 [u,2u,w] 0,x,1/6 [2u,u,w] x,x,5/6 [u,u,w]

6 g .2' x,0,0 [u,2u,w] 0,x,2/3 [2u,u,w] x,x,1/3 [u,u,w]

6 f .2' 1/2,0,z [u,v,0] 0,1/2,z+2/3 [v',u-v,0] 1/2,1/2,z+1/3 [u'+v',u',0]

6 e .2' 0,0,z [u,v,0] 0,0,z+2/3 [v',u-v,0] 0,0,z+1/3 [u'+v',u',0]

3 d 2'2' 1/2,0,1/2 [u,2u,0] 0,1/2,1/6 [2u,u,0] 1/2,1/2,5/6 [u,u,0]

3 c 2'2' 1/2,0,0 [u,2u,0] 0,1/2,2/3 [2u,u,0] 1/2,1/2,1/3 [u,u,0]

3 b 2'2' 0,0,1/2 [u,2u,0] 0,0,1/6 [2u,u,0] 0,0,5/6 [u,u,0]

3 a 2'2' 0,0,0 [u,2u,0] 0,0,2/3 [2u,u,0] 0,0,1/3 [u,u,0]

Symmetry of Special Projections

Along [0,0,1] p6m'm' Along [1,0,0] p2mm' Along [2,1,0] p2mm

\( a^* = a \quad b^* = b \)

Origin at 0,0,z

\( a^* = (a + 2b)/2 \quad b^* = c \)

Origin at x,0,0

\( a^* = c \quad b^* = b/2 \)

Origin at x,x/2,1/6

180.3.1398 - 2 - 3045
Origin at 22'2' at 6'2' (2,1,1) (1,2',1)

Asymmetric unit

\[
\begin{align*}
0 & \leq x \leq 1; & 0 & \leq y \leq 1; & 0 & \leq z \leq 1/6 & y & \leq x
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1,0,0 & & 1,1,0 \\
0,0,1/6 & & 1,0,1/6 & & 1,1,1/6
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1^*0,0,0) & \quad \text{Symmetry Operations} \\
\text{(2)} & \quad 3^* (0,0,2/3) & & 0,0,z \\
& \quad (3_2^*0,0,2/3) & & (3_2^*0,0,1/3) \\
(4) & \quad 2^* 0,0,z \\
& \quad (2_2^*0,0,0)^* & & (2_2^*0,0,0)^* \\
(5) & \quad 6^* (0,0,2/3) & & 0,0,z \\
& \quad (6_2^*0,0,2/3)^* & & (6_2^*0,0,1/3)^* \\
(7) & \quad 2^* x,x,1/3 \\
& \quad (2_2^*0,0,2/3) & & (2_2^*0,0,0) \\
(8) & \quad 2^* x,x,0 \\
& \quad (2_2^*0,0,0)^* & & (2_2^*0,0,0)^* \\
(9) & \quad 2^* x,2x,0 \\
& \quad (2_2^*0,0,0)^* & & (2_2^*0,0,0)^* \\
(10) & \quad 2^* x,x,1/3 \\
& \quad (2_2^*0,0,2/3) & & (2_2^*0,0,1/3) & & (2_2^*0,0,1/3) \\
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

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<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>12</td>
<td>k 1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z+2/3 [v,u-v,w] (3) x+y,x,z+1/3 [u+v,u,w] (4) x,y,z [u,v,w] (5) y,x+2/3 [v,u-v,w] (6) x,y,z+2/3 [v,u-v,w] (7) y,x,z [u,v,w] (8) x,y,z [u,v,w] (9) x+y,x,z+1/3 [u,u+v,w] (10) x+y,x,z+2/3 [u,u+v,w] (11) x+y,y,z [u,v,w] (12) x+y,x,z+1/3 [u,u+v,w]</td>
</tr>
<tr>
<td>6</td>
<td>j .2'</td>
<td>x,2x,1/2 [u,0,w] 2x,x,1/6 [0,u,w] x,x,5/6 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>i .2'</td>
<td>x,2x,0 [u,0,w] 2x,x,2/3 [0,u,w] x,x,1/3 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>h .2</td>
<td>x,0,1/2 [u,0,0] 0,x,1/6 [0,u,0] x,x,5/6 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>g .2</td>
<td>x,0,0 [u,0,0] 0,x,2/3 [0,u,0] x,x,1/3 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>f 2'..</td>
<td>0,1/2,z [u,v,0] 0,1/2,z+2/3 [v,u-v,0] 0,1/2,z+1/3 [v,u-v,0] 1/2,1/2,z+1/3 [u+v,u,0] 1/2,1/2,z+1/3 [u,v+u,0]</td>
</tr>
<tr>
<td></td>
<td>e 2'..</td>
<td>0,0,2 [u,v,0] 0,0,2+3 [v,u-v,0] 0,0,2+1/3 [u+v,u,0]</td>
</tr>
<tr>
<td></td>
<td>d 22'</td>
<td>1/2,0,1/2 [u,0,0] 0,1/2,1/6 [0,u,0] 1/2,1/2,5/6 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>c 22'</td>
<td>1/2,0,0 [u,0,0] 0,1/2,2/3 [0,u,0] 1/2,1/2,1/3 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>b 22'</td>
<td>0,0,1/2 [u,0,0] 0,0,1/6 [0,u,0] 0,0,5/6 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>a 22'</td>
<td>0,0,0 [u,0,0] 0,0,2/3 [0,u,0] 0,0,1/3 [u,u,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'mm'  
Along [1,0,0] p2mm  
Along [2,1,0] p2'mm'  

\( a^* = a \quad b^* = b \) 
\( a^* = c \quad b^* = (a + 2b)/2 \) 
\( a^* = b/2 \quad b^* = c \)
### Origin
at $2'2'2'$ at $6_2 (2',1,1) (1,2',1)$

### Asymmetric unit

- $0 \leq x \leq 1$
- $0 \leq y \leq 1$
- $0 \leq z \leq 1/6$
- $y \leq x$

### Vertices

- $0,0,0$
- $1,0,0$
- $1,1,0$
- $0,0,1/6$
- $1,0,1/6$
- $1,1,1/6$

### Symmetry Operations

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>$1$</td>
</tr>
<tr>
<td>(1)*0,0,0</td>
<td></td>
</tr>
<tr>
<td>(2) 3' (0,0,2/3)</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(3) 3' (0,0,1/3)</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(4) 2</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(2)*0,0,0</td>
<td></td>
</tr>
<tr>
<td>(5) 6 (0,0,2/3)</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(6) 6' (0,0,1/3)</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(7) 2' x,x,1/3</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(2,x)*0,0,2/3</td>
<td></td>
</tr>
<tr>
<td>(8) 2' x,0,0</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(2)*x0,0,0</td>
<td></td>
</tr>
<tr>
<td>(9) 2' 0,y,1/6</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(2,y)*0,0,1/3</td>
<td></td>
</tr>
<tr>
<td>(10) 2' x,x,1/3</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(2)*x0,0,2/3</td>
<td></td>
</tr>
<tr>
<td>(11) 2' x,2x,0</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(2)*x0,0,0</td>
<td></td>
</tr>
<tr>
<td>(12) 2' 2x,x,1/6</td>
<td>$0,0,z$</td>
</tr>
<tr>
<td>(2)*x0,0,1/3</td>
<td></td>
</tr>
</tbody>
</table>
**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**  

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<tbody>
<tr>
<td>12</td>
<td>k</td>
<td>(1) x,y,z [u,v,w] (2) y,x-z+2/3 [v,u-w] (3) x+y,z+1/3 [u+w,v]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u+v] (5) y,x+z+2/3 [v,u+w] (6) x-y,z+1/3 [u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x,z+2/3 [v,u+w] (8) x-y,x,z+1/3 [u+v,w] (9) x,y,z+1/3 [u+w,v]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) x+y,y,z, z+1/3 [u-v, w] (11) x+y,y,z [u+v, w] (12) x,y,z+1/3 [u+w, v]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p6mm</td>
</tr>
<tr>
<td>a* = a</td>
<td>Along [1,0,0]</td>
</tr>
<tr>
<td>b* = b</td>
<td>Along [2,1,0]</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>a* = c</td>
</tr>
<tr>
<td></td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td></td>
<td>Origin at x,x/2,1/6</td>
</tr>
</tbody>
</table>
**Symmetry Operations**

For \((0,0,0)\) + set

1. \(1\) \(\begin{pmatrix} 1^{*}\,0,0,0 \end{pmatrix}\)
2. \(3'\) \(\begin{pmatrix} 0,0,2/3 \end{pmatrix} 0,0,z\)
3. \(3'\) \(\begin{pmatrix} 0,0,1/3 \end{pmatrix} 0,0,z\)
4. \(2'\) \(\begin{pmatrix} 0,0,0 \end{pmatrix}\)
5. \(6'\) \(\begin{pmatrix} 0,0,2/3 \end{pmatrix} 0,0,z\)
6. \(6'\) \(\begin{pmatrix} 0,0,1/3 \end{pmatrix} 0,0,z\)
7. \(2\) \(\begin{pmatrix} x,x,1/6 \end{pmatrix}\)
8. \(2\) \(\begin{pmatrix} x,x,0 \end{pmatrix}\)
9. \(2'\) \(\begin{pmatrix} 0,y,1/2 \end{pmatrix} 0,y,1/2\)
10. \(2'\) \(\begin{pmatrix} 0,0,0 \end{pmatrix}\)
11. \(2'\) \(\begin{pmatrix} 0,0,0 \end{pmatrix}\)
12. \(2\) \(\begin{pmatrix} 2x,x,1/6 \end{pmatrix}\)

For \((0,0,1)\)' + set

1. \(1'\) \(\begin{pmatrix} 0,0,1 \end{pmatrix}\)
2. \(3'\) \(\begin{pmatrix} 0,0,5/3 \end{pmatrix} 0,0,z\)
3. \(3'\) \(\begin{pmatrix} 0,0,4/3 \end{pmatrix} 0,0,z\)
4. \(2\) \(\begin{pmatrix} 0,0,1 \end{pmatrix}\)
5. \(6\) \(\begin{pmatrix} 0,0,5/3 \end{pmatrix} 0,0,z\)
6. \(6\) \(\begin{pmatrix} 0,0,4/3 \end{pmatrix} 0,0,z\)
7. \(2'\) \(\begin{pmatrix} x,x,5/6 \end{pmatrix}\)
8. \(2'\) \(\begin{pmatrix} x,x,0 \end{pmatrix}\)
9. \(2\) \(\begin{pmatrix} 0,y,2/3 \end{pmatrix}\)
10. \(2\) \(\begin{pmatrix} 0,0,5/3 \end{pmatrix}\)
11. \(2\) \(\begin{pmatrix} 0,0,5/3 \end{pmatrix}\)
12. \(2'\) \(\begin{pmatrix} 0,y,2/3 \end{pmatrix}\)
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

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<tr>
<td>24</td>
<td>k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)' + (0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z+2/3 [v,u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z+1/3 [u-v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x, y,z [u,v,w]</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z+2/3 [v,u,v,w]</td>
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<td></td>
<td></td>
<td>(6) x-y,x,z+1/3 [u-v,u,w]</td>
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<td>(7) y,x,z+2/3 [v,u,w]</td>
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<td></td>
<td></td>
<td>(8) x-y,y,z [u-v,v,w]</td>
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<td>(9) x,x+y,z+1/3 [u-u,v,w]</td>
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<td>(10) y,x,z+2/3 [v,u,w]</td>
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<td>(11) x+y,y,z [u-v,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(12) x,x-y,z+1/3 [u-u,v,w]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6mm1'

a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p222' 2m'm'

a* = c  b* = (a + 2b)/2
Origin at x,0,0

Along [2,1,0] p222' 2m'm'

a* = c  b* = b/2
Origin at x,x/2,1/6

180.6.1401 - 2 - 3051
**Origin** at 222' at 6_2' (2,1,1) (1,2,1)

**Asymmetric unit**

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6\]

Vertices

- \(0,0,0\)
- \(1,0,0\)
- \(1,1,0\)
- \(0,0,1/6\)
- \(1,0,1/6\)
- \(1,1,1/6\)

**Symmetry Operations**

For \((0,0,0) + \) set

1. \(1 (1^{*}0,0,0)\)
2. \(3' (0,0,2/3) 0,0,z\)
3. \(3' (0,0,1/3) 0,0,z\)
4. \(2 z^*0,0,0\)
5. \(6 (0,0,2/3) 0,0,z\)
6. \(6 (0,0,1/3) 0,0,z\)
7. \(2 x,x,1/3 (2,0,0,2/3)\)
8. \(2 (0,0,0) x,0,0\)
9. \(2' (0,0,1/3) 0,0,1/2\)
10. \(2 x,0,1/2 (2,0,0,2/3)\)
11. \(2 x,x,1/3 (2,0,0,2/3)\)
12. \(2' (0,0,1/3) 0,0,1/2\)

For \((0,0,1) + \) set

1. \(1' (0,0,1) (1^{*}0,0,0)\)
2. \(3' (0,0,5/3) 0,0,z\)
3. \(3' (0,0,4/3) 0,0,z\)
4. \(2' (0,0,1) (2,0,0,1)\)
5. \(6' (0,0,5/3) 0,0,z\)
6. \(6' (0,0,4/3) 0,0,z\)
7. \(2 x,x,5/6 (2,0,0,5/3)\)
8. \(2 (0,0,1) x,0,1/2\)
9. \(2' (0,0,1) 0,0,2/3\)
10. \(2' (0,0,1) 2x,x,1/2\)
11. \(2' (0,0,1) 2x,x,1/2\)
12. \(2 (2,0,0,4/3) 0,0,1/2\)

**180.7.1402**
Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' +</td>
<td></td>
</tr>
<tr>
<td>24 k 1</td>
<td>(1) x,y,z [u,v,w] (2) y,-x-y,z+2/3 [v,u-v,w] (3) x+y,x,z+1/3 [u-v,u,w] (4) x,-y,z [u,v,w] (5) x,-y,z+2/3 [v,u-v,w] (6) x,-y,x,z+1/3 [u-v,u,w] (7) x,y,z [u,v,w] (8) x,y,z+2/3 [v,u-v,w] (9) x,-y,x,z+1/3 [u-v,u,w] (10) x,y,z [u,v,w] (11) x+y,x,z [u+v,v,w] (12) x,y,z [u,v,w] (13) x+y,x,z+1/3 [u+v,u,w]</td>
</tr>
<tr>
<td>12 j ..2'</td>
<td>x,2x,1/2 [u,0,w] 2x,x,1/6 [0,u,w] x,x,5/6 [u,u,w]</td>
</tr>
<tr>
<td>12 i ..2</td>
<td>x,2x,0 [u,2u,0] 2x,x,2/3 [2u,u,0] x,x,1/3 [u,u,0]</td>
</tr>
<tr>
<td>12 h ..2'</td>
<td>x,0,1/2 [u,2u,w] 0,x,1/6 [2u,u,0] x,x,5/6 [u,u,w]</td>
</tr>
<tr>
<td>12 g ..2</td>
<td>x,0,0 [u,0,0] 0,x,2/3 [0,u,0] x,x,1/3 [u,u,0]</td>
</tr>
<tr>
<td>12 f ..2</td>
<td>1/2,0,z [0,0,w] 0,1/2,z+2/3 [0,0,w] 1/2,1/2,z+1/3 [0,0,w]</td>
</tr>
<tr>
<td>12 e ..2</td>
<td>0,0,z [0,0,w] 0,0,z+2/3 [0,0,w] 0,0,z+1/3 [0,0,w]</td>
</tr>
<tr>
<td>6 d 2'2</td>
<td>1/2,0,1/2 [0,0,w] 0,1/2,1/6 [0,0,w] 1/2,1/2,5/6 [0,0,w]</td>
</tr>
<tr>
<td>6 c 222</td>
<td>1/2,0,0 [0,0,0] 0,1/2,2/3 [0,0,0] 1/2,1/2,1/3 [0,0,0]</td>
</tr>
<tr>
<td>6 b 2'2'</td>
<td>0,0,1/2 [0,0,w] 0,0,1/6 [0,0,w] 0,0,5/6 [0,0,w]</td>
</tr>
<tr>
<td>6 a 222</td>
<td>0,0,0 [0,0,0] 0,0,2/3 [0,0,0] 0,0,1/3 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6mm1' 
Along [1,0,0] p2a2' 2mm 
Along [2,1,0] p2a2' 2mm 

\[ a^* = a \hspace{1cm} b^* = b \]

Origin at 0,0,z 
Origin at x,0,0 
Origin at x,x/2,2/3
Origin at 222 at $6_g (2,1,1) (1,2,1)$

Asymmetric unit

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{6}\]

Vertices:

- 0,0,0
- 1,0,0
- 1,1,0
- 0,0,\frac{1}{6}
- 1,0,\frac{1}{6}
- 1,1,\frac{1}{6}

Symmetry Operations

1. \((1) 1\)
2. \((1) 0,0,0\)
3. \((1) 3 (0,0,1/3) 0,0,z\)
4. \((3_z 0,0,1/3)\)
5. \((3) 3^* (0,0,2/3) 0,0,z\)
6. \((3_z^{-1} 0,0,2/3)\)
7. \((4) 2 0,0,z\)
8. \((2_z 0,0,0)\)
9. \((2_z) 0,0,0\)
10. \((2_z) 0,0,0\)
11. \((2_z 0,0,2/3)\)
12. \((2_z 0,0,2/3)\)

\(181.1.1403\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
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<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
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</thead>
<tbody>
<tr>
<td>12 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(7) y,x,z+1/3 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/3 [v,u,w]</td>
</tr>
<tr>
<td>6 j .2</td>
<td>x,2x,1/2 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td>x,2x,1/2 [u,2u,0]</td>
</tr>
<tr>
<td>6 i .2</td>
<td>x,2x,0 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td>x,2x,0 [u,2u,0]</td>
</tr>
<tr>
<td>6 h .2</td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>6 g .2</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>6 f 2..</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/3 [0,0,w]</td>
</tr>
<tr>
<td>6 e 2..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/3 [0,0,w]</td>
</tr>
<tr>
<td>3 d 222</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 c 222</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>3 b 222</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 a 222</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6m' m'  
\( a^* = a \) \( b^* = b \)  
Origin at 0,0,z

Along [1,0,0] p2m' m'  
\( a^* = c \) \( b^* = (a + 2b)/2 \)  
Origin at x,0,0

Along [2,1,0] p2m' m'  
\( a^* = c \) \( b^* = b/2 \)  
Origin at x,x/2,1/3
Origin at 2221' at 64 (2,1,1) (1,2,1)1'

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq \frac{1}{6}; \quad y \leq x \]

Vertices

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1,0,0</th>
<th>1,1,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
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</tr>
</tbody>
</table>

Symmetry Operations

For 1 + set

(1) 1
(1 | 0,0,0)

(4) 2
(2 | 0,0,z)

(5) 6'
(6 | 0,0,1/3)

(7) 2
(2y | 0,0,1/3)

(10) 2
(2 | x,x,1/6)

(8) 2
(2 | x,0,0)

(9) 2
(2 | 0,y,1/3)

(12) 2
(2 | 0,0,2/3)

(11) 2
(2 | x,2x,0)

(2 | 0,0,0)
For $1'$ + set

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 k</td>
<td>11'</td>
<td>(1) x,y,z [0,0,0]</td>
<td>$1'$ + $1'$ +</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) $y$,x-y,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) $x$, $y$,z [0,0,0]</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z+1/3 [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>(7) y,x,z+1/3 [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>(10) $y$, $x$,z+1/3 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>6 j</td>
<td>..21'</td>
<td>x,2x,1/2 [0,0,0]</td>
<td>2x, $x$,5/6 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$x$,2x,1/2 [0,0,0]</td>
<td>2x,$x$,5/6 [0,0,0]</td>
</tr>
<tr>
<td>6 i</td>
<td>..21'</td>
<td>x,2x,0 [0,0,0]</td>
<td>2x,$x$,1/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,0 [0,0,0]</td>
<td>2x,$x$,1/3 [0,0,0]</td>
</tr>
<tr>
<td>6 h</td>
<td>.21'</td>
<td>x,0,1/2 [0,0,0]</td>
<td>0,$x$,5/6 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$x$,0,1/2 [0,0,0]</td>
<td>0,$x$,5/6 [0,0,0]</td>
</tr>
<tr>
<td>6 g</td>
<td>.21'</td>
<td>x,0,0 [0,0,0]</td>
<td>0,$x$,1/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$x$,0,0 [0,0,0]</td>
<td>0,$x$,1/3 [0,0,0]</td>
</tr>
<tr>
<td>6 f</td>
<td>2..1'</td>
<td>1/2,0,z [0,0,0]</td>
<td>0,1/2,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,$z$,+1/3 [0,0,0]</td>
<td>1/2,0,$z$ [0,0,0]</td>
</tr>
<tr>
<td>6 e</td>
<td>2..1'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/3 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+1/3 [0,0,0]</td>
<td>0,0,$z$ [0,0,0]</td>
</tr>
<tr>
<td>3 d</td>
<td>2221'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,5/6 [0,0,0]</td>
</tr>
</tbody>
</table>
Continued

| 3 | c | 2221' | 1/2,0,0 [0,0,0] | 0,1/2,1/3 [0,0,0] | 1/2,1/2,2/3 [0,0,0] |
| 3 | b | 2221' | 0,0,1/2 [0,0,0] | 0,0,5/6 [0,0,0] | 0,0,1/6 [0,0,0] |
| 3 | a | 2221' | 0,0,0 [0,0,0] | 0,0,1/3 [0,0,0] | 0,0,2/3 [0,0,0] |

Symmetry of Special Projections

| Along [0,0,1] | p6mm1' | a* = a b* = b | a* = a b* = (a + 2b)/2 |
| Origin at 0,0,z | | Origin at x,0,0 | |

| Along [1,0,0] | p2mm1' | a* = c b* = (a + 2b)/2 |
| Origin at x,x/2,1/3 | | |

| Along [2,1,0] | p2mm1' | a* = c b* = b/2 |
| Origin at x,x/2,1/3 | | |
**Origin** at 2'2'2' at 6'2' (2',1,1) (1,2,1)

**Asymmetric unit**

<table>
<thead>
<tr>
<th></th>
<th>0 ≤ x ≤ 1;</th>
<th>0 ≤ y ≤ 1;</th>
<th>0 ≤ z ≤ 1/6</th>
<th>y ≤ x</th>
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<tbody>
<tr>
<td>Vertices</td>
<td>0,0,0</td>
<td>1,0,0</td>
<td>1,1,0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. 1
   - \(1|0,0,0\)
2. 3' (0,0,1/3) 0,0,z
   - \(3_z|0,0,1/3\)
3. 3' (0,0,2/3) 0,0,z
   - \(3_z^{-1}|0,0,2/3\)
4. 2' 0,0,z
   - \(2|0,0,0\)
   - \(2|0,0,0\)'
5. 6' (0,0,1/3) 0,0,z
   - \(6_z|0,0,1/3\')
6. 6' (0,0,2/3) 0,0,z
   - \(6_z|0,0,2/3\')
7. 2' x,x,1/6
   - \(2_x|0,0,1/3\)
   - \(2_x|0,0,1/3\)'
8. 2' x,0,0
   - \(2_x|0,0,0\)
   - \(2_x|0,0,0\)'
9. 2' 0,y,1/3
   - \(2_y|0,0,2/3\)
   - \(2_y|0,0,2/3\')
10. 2 x,x,1/6
    - \(2|0,0,1/3\)
11. 2 x,2x,0
    - \(2|0,0,0\)
12. 2 2x,x,1/3
    - \(2|0,0,2/3\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>k</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) (\vec{y},-x-y,\vec{z}+1/3 [\vec{v},u-v,w] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) (x+y,\vec{x},\vec{z}+2/3 [\vec{u}+v,\vec{u},w] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) (\vec{x},\vec{y},\vec{z} [u,v,w] )</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(5) (y,x+y,\vec{z}+1/3 [\vec{v},u-v,w] )</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(6) (x-y,x,\vec{z}+2/3 [\vec{u}+v,\vec{u},w] )</td>
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<td></td>
<td>(7) (y,x,\vec{z}+1/3 [v,u,w] )</td>
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<td>(8) (x-y,\vec{y},\vec{z} [u+v,v,w] )</td>
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<td>(9) (x,\vec{x}+y,\vec{z}+2/3 [u-u-v,w] )</td>
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<td>(10) (\vec{y},\vec{x},\vec{z}+1/3 [v,u,w] )</td>
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<td>(11) (\vec{x}+y,\vec{y},\vec{z} [u+v,v,w] )</td>
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<td></td>
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<td>(12) (\vec{x}-y,\vec{x},\vec{z}+2/3 [u-u-v,w] )</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>.2</td>
<td>x,2x,1/2 [u,2u,0]</td>
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<td></td>
<td>(2\vec{x},\vec{x},5/6 [2\vec{u},\vec{u},0] )</td>
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<td></td>
<td></td>
<td>(x,\vec{x},1/6 [u,\vec{u},0] )</td>
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<td></td>
<td></td>
<td>(\vec{x},2\vec{x},1/2 [u,2u,0] )</td>
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<td>(2\vec{x},\vec{x},5/6 [2\vec{u},\vec{u},0] )</td>
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<td></td>
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<td>(x,\vec{x},1/6 [u,\vec{u},0] )</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>.2</td>
<td>x,2x,0 [u,2u,0]</td>
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<td>(2\vec{x},\vec{x},1/3 [2\vec{u},\vec{u},0] )</td>
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<td>.2'</td>
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<td>g</td>
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<td>(\vec{x},0,0 [u,2u,\vec{w}] )</td>
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<tr>
<td>6</td>
<td>f</td>
<td>.2'</td>
<td>(1/2,0,\vec{z} [\vec{u},v,\vec{w}] )</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(0,1/2,\vec{z}+1/3 [\vec{v},u-v,\vec{w}] )</td>
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<td>(1/2,1/2,\vec{z}+2/3 [u+v,\vec{u},\vec{w}] )</td>
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<td></td>
<td>(0,1/2,\vec{z}+1/3 [v,u,\vec{w}] )</td>
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<td>(1/2,0,\vec{z}+1/3 [\vec{u}+v,v,\vec{w}] )</td>
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<td>(1/2,1/2,\vec{z}+2/3 [u,u-v,\vec{w}] )</td>
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<tr>
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<td>e</td>
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<td>(0,0,\vec{z} [\vec{u},v,\vec{w}] )</td>
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<td>(0,0,\vec{z}+1/3 [\vec{v},u-v,\vec{w}] )</td>
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<td>(0,0,\vec{z}+1/3 [\vec{v},u,\vec{w}] )</td>
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<td>(0,0,\vec{z} [\vec{u}+v,v,\vec{w}] )</td>
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<td>(0,0,\vec{z}+2/3 [u,u-v,\vec{w}] )</td>
</tr>
<tr>
<td>3</td>
<td>d</td>
<td>2'2'</td>
<td>(1/2,0,1/2 [u,2u,0] )</td>
</tr>
<tr>
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<td></td>
<td></td>
<td>(0,1/2,5/6 [2\vec{u},\vec{u},0] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(1/2,1/2,1/6 [\vec{u},\vec{u},0] )</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>2'2'</td>
<td>(1/2,0,0 [u,2u,0] )</td>
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<td></td>
<td></td>
<td></td>
<td>(0,1/2,1/3 [2\vec{u},\vec{u},0] )</td>
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<tr>
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<td></td>
<td></td>
<td>(1/2,1/2,2/3 [\vec{u},\vec{u},0] )</td>
</tr>
<tr>
<td>3</td>
<td>b</td>
<td>2'2'</td>
<td>(0,0,1/2 [u,2u,0] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0,0,5/6 [2\vec{u},\vec{u},0] )</td>
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<td></td>
<td></td>
<td></td>
<td>(0,0,1/6 [u,\vec{u},0] )</td>
</tr>
<tr>
<td>3</td>
<td>a</td>
<td>2'2'</td>
<td>(0,0,0 [u,2u,0] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0,0,1/3 [2\vec{u},\vec{u},0] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0,0,2/3 [\vec{u},\vec{u},0] )</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6m'</th>
<th>a = a</th>
<th>b = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,0,0]</td>
<td>p2mm</td>
<td>a = c</td>
<td>b = (a + 2b)/2</td>
</tr>
<tr>
<td>Along [2,1,0]</td>
<td>p2mm</td>
<td>a = c</td>
<td>b = b/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x/2,1/3

181.3.1405 - 2 - 3060
Origin at 22'2' at 6' (2,1,1) (1,2',1)

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \quad y \leq x \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1,1,0 \\
0,0,1/6 & \quad 1,0,1/6 & \quad 1,1,1/6
\end{align*}
\]

Symmetry Operations

1. \(1\)
   \[
   (1 | 0,0,0)
   \]

2. \(3'\)
   \[
   (0,0,1/3) \quad 0,0,z \\
   (3_z | 0,0,1/3)
   \]

3. \(3'\)
   \[
   (0,0,2/3) \quad 0,0,z \\
   (3_z^{-1} | 0,0,2/3)
   \]

4. \(2'\)
   \[
   0,0,Z \\
   (2_z | 0,0,0)
   \]

5. \(6'\)
   \[
   (0,0,1/3) \quad 0,0,z \\
   (6_z^{-1} | 0,0,1/3)
   \]

6. \(6'\)
   \[
   (0,0,2/3) \quad 0,0,z \\
   (6_z | 0,0,2/3)
   \]

7. \(2\)
   \[
   x,x,1/6 \\
   (2_x | 0,0,1/3)
   \]

8. \(2\)
   \[
   x,0,0 \\
   (2_x | 0,0,0)
   \]

9. \(2\)
   \[
   0,y,1/3 \\
   (2_y | 0,0,2/3)
   \]

10. \(2'\)
    \[
    x,x,1/6 \\
    (2_z | 0,0,1/3)
    \]

11. \(2'\)
    \[
    x,2x,0 \\
    (2_z | 0,0,0)
    \]

12. \(2'\)
    \[
    2x,x,1/3 \\
    (2_z | 0,0,2/3)
    \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>k</td>
<td>1</td>
</tr>
<tr>
<td>(1) x,y,z</td>
<td>u,v,w</td>
<td>(2) y,x-y,z+1/3 [v,u-v,w]</td>
</tr>
<tr>
<td>(4) x,y,z</td>
<td>u,v,w</td>
<td>(3) x+y,x,z+2/3 [u+v,u,w]</td>
</tr>
<tr>
<td>(7) y,x,z</td>
<td>v,u,w</td>
<td></td>
</tr>
<tr>
<td>(10) y,x,z</td>
<td>v,u,w</td>
<td></td>
</tr>
</tbody>
</table>

| 6             | j              | .2             |
| 1/2,0,z      | [u,v,0]        | 1/2,1/2,1/3 [u+v,u,v] |
|               |                |               |
| 6             | i              | .2             |
| 1/2,0,z      | [u,v,0]        | 1/2,1/2,1/3 [u+v,u,v] |

| 6             | h              | .2             |
| 1/2,0,z      | [u,v,0]        | 1/2,1/2,1/3 [u+v,u,v] |

| 6             | g              | .2             |
| 1/2,0,z      | [u,v,0]        | 1/2,1/2,1/3 [u+v,u,v] |

Symmetry of Special Projections

Along [0,0,1] p6mm'  
\[ a^* = a \quad b^* = b \]  
Origin at 0,0,z

Along [1,0,0] p2mm  
\[ a^* = c \quad b^* = (a + 2b)/2 \]  
Origin at x,0,0

Along [2,1,0] p2mm'  
\[ a^* = b/2 \quad b^* = c \]  
Origin at x,x/2,1/3
Origin at 2'2'2' at 6_4 (2',1,1) (1,2',1)

Asymmetric unit

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0,0,0</th>
<th>1,0,0</th>
<th>1,1,0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0,0,1/6</td>
<td>1,0,1/6</td>
<td>1,1,1/6</td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 3' (0,0,1/3) 0,0,z
(3 z | 0,0,1/3)

(4) 2 0,0,z
(2 | 0,0,0)

(5) 6' (0,0,1/3) 0,0,z
(6 z | 0,0,1/3)

(7) 2' x,x,1/6
(2y | 0,0,1/3)

(8) 2' x,0,0
(2y | 0,0,0)

(9) 2' 0,y,1/3
(2z | 0,0,2/3)

(10) 2' x,x,1/6
(2z | 0,0,1/3)

(11) 2' x,2x,0
(2y | 0,0,0)

(12) 2' 2x,x,1/3
(2z | 0,0,2/3)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>k 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z+1/3 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) x, y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(7) y,x,z+1/3 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(10) y, x-z+1/3 [v,u,w]</td>
</tr>
<tr>
<td>6</td>
<td>j ..2'</td>
<td>x,2x,1/2 [u,0,w]</td>
<td>2x,2x,1/2 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,5/6 [0,u,w]</td>
<td>2x,5/6 [0,u,w]</td>
</tr>
<tr>
<td></td>
<td>i ..2'</td>
<td>x,2x,0 [u,0,w]</td>
<td>2x,2x,0 [u,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,1/3 [0,u,w]</td>
<td>2x,1/3 [0,u,w]</td>
</tr>
<tr>
<td></td>
<td>h .2'.</td>
<td>x,0,1/2 [u,2u,w]</td>
<td>0,5/6 [2u,0,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2 [u,2u,w]</td>
<td>0,1/2 [u,2u,w]</td>
</tr>
<tr>
<td></td>
<td>g .2'.</td>
<td>x,0,0 [u,2u,w]</td>
<td>0,1/3 [2u,0,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0 [u,2u,w]</td>
<td>0,0 [u,2u,w]</td>
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<tr>
<td></td>
<td>f 2..</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
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<tr>
<td></td>
<td></td>
<td>1/2,0,z+1/3 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
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<tr>
<td></td>
<td>e 2..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/3 [0,0,w]</td>
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<tr>
<td></td>
<td></td>
<td>0,0,z+1/3 [0,0,w]</td>
<td>0,0,z+1/3 [0,0,w]</td>
</tr>
<tr>
<td>3</td>
<td>d 22'2'</td>
<td>1/2,0,1/2 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>c 22'2'</td>
<td>1/2,0,0 [0,0,w]</td>
<td>1/2,1/2,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>b 22'2'</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,5/6 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>a 22'2'</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,1/3 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm</th>
<th>Along [1,0,0]</th>
<th>p2'2mm'</th>
<th>Along [2,1,0]</th>
<th>p2'2mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a' = a</td>
<td>b' = b</td>
<td>a' = c</td>
<td>b' = (a + 2b)/2</td>
<td>a' = c</td>
<td>b' = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,1/3</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at 222 at 6\textsubscript{a} (2,1,1) (1,2,1)

**Asymmetric unit**

\begin{align*}
0 &\leq x \leq 1; \\
0 &\leq y \leq 1; \\
0 &\leq z \leq 1/6 \\
y &\leq x
\end{align*}

**Vertices**

\begin{align*}
0,0,0 &\quad 1,0,0 &\quad 1,1,0 \\
0,0,1/6 &\quad 1,0,1/6 &\quad 1,1,1/6
\end{align*}

**Symmetry Operations**

For (0,0,0) + set

\begin{align*}
(1) &\quad 1 &\quad (2) &\quad 3' (0,0,1/3) &\quad 0,0,z \\
\quad (1|0,0,0) &\quad (3) &\quad 3' (0,0,2/3) &\quad 0,0,z \\
\quad (3|0,0,2/3) &\quad (3|0,0,1/3)' &\quad (3|0,0,2/3) &\quad (3|0,0,1/3)'
\end{align*}

\begin{align*}
(4) &\quad 2 0,0,z &\quad (5) &\quad 6' (0,0,1/3) &\quad 0,0,z \\
\quad (2|0,0,0) &\quad (6) &\quad 6' (0,0,2/3) &\quad 0,0,z \\
\quad (6|0,0,2/3) &\quad (6|0,0,1/3)' &\quad (6|0,0,2/3) &\quad (6|0,0,1/3)'
\end{align*}

\begin{align*}
(7) &\quad 2' x,x,1/6 &\quad (8) &\quad 2 x,0,0 \\
\quad (2|0,0,1/3)' &\quad (2|0,0,0) &\quad (9) &\quad 2 0,y,1/3 \\
\quad (2|0,0,2/3) &\quad (2|0,0,0) &\quad (2|0,0,2/3) &\quad (2|0,0,1/3)
\end{align*}

\begin{align*}
(10) &\quad 2' x,x,1/6 &\quad (11) &\quad 2 x,2x,0 \\
\quad (2|0,0,1/3)' &\quad (2|0,0,0) &\quad (12) &\quad 2 2x,x,1/3 \\
\quad (2|0,0,1/3)' &\quad (2|0,0,0) &\quad (2|0,0,2/3) &\quad (2|0,0,1/3)'
\end{align*}
Continued

For \((0,0,1)\)' + set

<table>
<thead>
<tr>
<th>(1) (t' (0,0,1))</th>
<th>(2) (3' (0,0,4/3))</th>
<th>(3) (3' (0,0,5/3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1 {0,0,1}')</td>
<td>(0,0,z) ((0,0,4/3))</td>
<td>(0,0,z) ((0,0,5/3))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) (2' (0,0,1))</th>
<th>(5) (6' (0,0,4/3))</th>
<th>(6) (6' (0,0,5/3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2 {0,0,1}')</td>
<td>(0,0,z) ((0,0,4/3))</td>
<td>(0,0,z) ((0,0,5/3))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) (2 x,2/3)</th>
<th>(8) (x,0,1/2)</th>
<th>(9) (0,y,5/6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2{0,0,4/3})</td>
<td>(2{0,0,1}')</td>
<td>(2{0,0,5/3}')</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) (2 x,2/3)</th>
<th>(11) (2' x,2,1/2)</th>
<th>(12) (2' 2x,5/6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2{0,0,4/3})</td>
<td>(2{0,0,1}')</td>
<td>(2{0,0,5/3}')</td>
</tr>
</tbody>
</table>

**Generators selected**

(1); \(t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + ((0,0,1)' +)</td>
<td>(0,0,0) + ((0,0,1)' +)</td>
</tr>
<tr>
<td>(24 k 1)</td>
<td>(x,y,z [u,v,w])</td>
</tr>
<tr>
<td></td>
<td>(y,x-y,z+1/3 [v,u-v,w])</td>
</tr>
<tr>
<td></td>
<td>(x+y,x,z+2/3 [u+v,u,w])</td>
</tr>
<tr>
<td></td>
<td>(x,y,z [u,v+w])</td>
</tr>
<tr>
<td></td>
<td>(y,x+vy,z+1/3 [v,u+v,w])</td>
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<td>(x+y,x,z+2/3 [u+v,u+w])</td>
</tr>
<tr>
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<td>(x+y,x,z+1/3 [u+v,w])</td>
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<tr>
<td></td>
<td>(x,x,1/2 [u,0,0])</td>
</tr>
<tr>
<td></td>
<td>(0,x,5/6 [2u,u,w])</td>
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<td></td>
<td>(x,x,1/6 [u,u,w])</td>
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<td>(x,x,1/3 [2u,u,0])</td>
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<td>(x,x,1/3 [2u,u,0])</td>
</tr>
<tr>
<td></td>
<td>(x,x,2/3 [u,u,0])</td>
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</tbody>
</table>

**Positions**

**Generators selected**

(1); \(t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).
Continued

Symmetry of Special Projections

Along [0,0,1] p6mm1'  
\( a^* = a \quad b^* = b \)  
Origin at 0,0,z

Along [1,0,0] \( p_{2a'} \cdot 2m'm' \)  
\( a^* = c \quad b^* = (a + 2b)/2 \)  
Origin at x,0,0

Along [2,1,0] \( p_{2a} \cdot 2m'm' \)  
\( a^* = c \quad b^* = b/2 \)  
Origin at x,x/2,1/3

6 \hspace{1em} c \hspace{1em} 222 \hspace{1em} 1/2,0,0 [0,0,0] \hspace{1em} 0,1/2,1/3 [0,0,0] \hspace{1em} 1/2,1/2,2/3 [0,0,0]

6 \hspace{1em} b \hspace{1em} 22'2' \hspace{1em} 0,0,1/2 [u,2u,0] \hspace{1em} 0,0,5/6 [2u, u,0] \hspace{1em} 0,0,1/6 [u,u,0]

6 \hspace{1em} a \hspace{1em} 222 \hspace{1em} 0,0,0 [0,0,0] \hspace{1em} 0,0,1/3 [0,0,0] \hspace{1em} 0,0,2/3 [0,0,0]
Origin at $2'22'$ at $6_3' (2',1,1) (1,2,1)$

Asymmetric unit: $0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/6 \quad y \leq x$

Vertices: $0,0,0; \quad 1,0,0; \quad 1,1,0$
$0,0,1/6; \quad 1,0,1/6; \quad 1,1,1/6$

Symmetry Operations

For $(0,0,0)$ + set

(1) $1$

(2) $3^* (0,0,1/3) \quad 0,0,z$
$3_2^* (0,0,1/3)'$

(3) $3^*(0,0,2/3) \quad 0,0,z$
$3_2^* (0,0,2/3)$

(4) $2' \quad 0,0,z$
$2_2 (0,0,0)'$

(5) $6 (0,0,1/3) \quad 0,0,z$
$6_2^* (0,0,1/3)$

(6) $6^* (0,0,2/3) \quad 0,0,z$
$6_2^* (0,0,2/3)'$

(7) $2 \quad x,x,1/6$
$2_{yx} (0,0,1/3)$

(8) $2' \quad x,0,0$
$2_2 (0,0,0)'$

(9) $2' \quad 0,y,1/3$
$2_2 (0,0,2/3)'$

(10) $2' \quad x,x,1/6$
$2_{yx} (0,0,1/3)'$

(11) $2 \quad x,2x,0$
$2_2 (0,0,0)$

(12) $2 \quad 2x,x,1/3$
$2_2 (0,0,2/3)$
Continued

For \((0,0,1)'+\) set

\[
\begin{align*}
(1) & \quad t' \quad (0,0,1) \\
(2) & \quad 3' \quad (0,0,4/3) \\
(3) & \quad 3' \quad (0,0,5/3) \\
(4) & \quad 2 \quad (0,0,1) \\
(5) & \quad 6' \quad (0,0,4/3) \\
(6) & \quad 6' \quad (0,0,5/3) \\
(7) & \quad 2' \quad x,x,2/3 \\
(8) & \quad 2' \quad x,0,1/2 \\
(9) & \quad 2' \quad 0,y,5/6 \\
(10) & \quad 2 \quad x,x,2/3 \\
(11) & \quad 2' \quad x,2x,1/2 \\
(12) & \quad 2' \quad 2x,x,5/6
\end{align*}
\]

\[\]

Generators selected \((1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(24)</td>
<td>((0,0,0) + (0,0,1)'+)</td>
</tr>
<tr>
<td>(k)</td>
<td>((1) x,y,z [u,v,w] )</td>
</tr>
<tr>
<td>(j)</td>
<td>((2) \bar{y},x-y,z+1/3 [v,u-v,w] )</td>
</tr>
<tr>
<td>(l)</td>
<td>((3) x+y,x,z+2/3 [u+v,\bar{u},w] )</td>
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<tr>
<td>(i)</td>
<td>((4) \bar{x},y,z [u,v,w] )</td>
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<tr>
<td>(m)</td>
<td>((5) y,x+y,z+1/3 [v,u-v,w] )</td>
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<tr>
<td>(n)</td>
<td>((6) x-y,x,z+2/3 [u+v,\bar{u},w] )</td>
</tr>
<tr>
<td>(h)</td>
<td>((7) y,x,z+1/3 [v,\bar{u},w] )</td>
</tr>
<tr>
<td>(k)</td>
<td>((8) \bar{x},y,\bar{z} [u+v,v,w] )</td>
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<tr>
<td>(l)</td>
<td>((9) \bar{x},x+y,\bar{z}+2/3 [u-u,v,w] )</td>
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<tr>
<td>(g)</td>
<td>((10) \bar{y},x+z+1/3 [v,\bar{u},w] )</td>
</tr>
<tr>
<td>(h)</td>
<td>((11) \bar{x}+y,y,\bar{z}+2/3 [u+v,v,w] )</td>
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<tr>
<td>(f)</td>
<td>((12) x,x-y,\bar{z}+2/3 [u,u-v,\bar{w}] )</td>
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<tr>
<td>(e)</td>
<td>((13) x,0,1/2 [u,0,0] )</td>
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<td>(d)</td>
<td>((14) \bar{x},0,1/2 [u,0,0] )</td>
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<tr>
<td>(c)</td>
<td>((15) 0,x,5/6 [0,u,0] )</td>
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<tr>
<td>(b)</td>
<td>((16) \bar{x},0,5/6 [0,u,0] )</td>
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<tr>
<td>(a)</td>
<td>((17) 0,0,1/2 [u,0,0] )</td>
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<tr>
<td></td>
<td>((18) 0,0,5/6 [0,u,0] )</td>
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<tr>
<td></td>
<td>((19) 0,0,1/2 [u,0,0] )</td>
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<tr>
<td></td>
<td>((20) 0,0,5/6 [0,u,0] )</td>
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<tr>
<td></td>
<td>((21) 0,0,1/2 [u,0,0] )</td>
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<tr>
<td></td>
<td>((22) 0,0,5/6 [0,u,0] )</td>
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<table>
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<tr>
<th></th>
<th>6</th>
<th>c</th>
<th>2'2'</th>
<th>1/2,0,0 [u,2u,0]</th>
<th>0,1/2,1/3 [2u, u, 0]</th>
<th>1/2,1/2,2/3 [u, u, 0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>6</td>
<td>b</td>
<td>2'2'</td>
<td>0,0,1/2 [u,0,0]</td>
<td>0,0,1/6 [0,0,0]</td>
<td>0,0,1/6 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>a</td>
<td>2'2'</td>
<td>0,0,0 [u,2u,0]</td>
<td>0,0,1/3 [2u, u, 0]</td>
<td>0,0,2/3 [u, u, 0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] \( p6_{mm} \)

- \( \mathbf{a}^* = \mathbf{a} \)
- \( \mathbf{b}^* = \mathbf{b} \)

Origin at 0,0,z

Along [1,0,0] \( p_{2a}^{2mm} \)

- \( \mathbf{a}^* = \mathbf{c} \)
- \( \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)

Origin at x,0,1/2

Along [2,1,0] \( p_{2a}^{2mm} \)

- \( \mathbf{a}^* = \mathbf{c} \)
- \( \mathbf{b}^* = \mathbf{b}/2 \)

Origin at x,x/2,1/3
**Origin** at 321 at 6₃21

**Asymmetric unit**

\[0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)\]

**Vertices**

\[
\begin{array}{cccccc}
0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/3,2/3,0 & 0,1/2,0 \\
0,0,1/4 & 1/2,0,1/4 & 2/3,1/3,1/4 & 1/3,2/3,1/4 & 0,1/2,1/4 \\
\end{array}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) \ & \ 1 \\
(1) \ & \ 1 \quad 0,0,0 \\
(1) \ & \ 0,0,0 \\
(4) \ & \ 2 \quad (0,0,1/2) \quad 0,0,z \\
(2,0,0,1/2) \ & \ (2,0,0,1/2) \\
(5) \ & \ 6 \quad (0,0,1/2) \quad 0,0,z \\
(6,1,0,1/2) \ & \ (6,1,0,1/2) \\
(7) \ & \ 2 \quad x,x,0 \\
\quad (2_x,0,0,0) \ & \ (2_x,0,0,0) \\
(8) \ & \ 2 \quad x,0,0 \\
\quad (2,0,0,0) \ & \ (2,0,0,0) \\
(9) \ & \ 2 \quad 0,y,0 \\
\quad (2_y,0,0,0) \ & \ (2_y,0,0,0) \\
(10) \ & \ 2 \quad x,1/4 \\
\quad (2,0,0,1/2) \ & \ (2,0,0,1/2) \\
(11) \ & \ 2 \quad x,2,1/4 \\
\quad (2,0,0,1/2) \ & \ (2,0,0,1/2) \\
(12) \ & \ 2 \quad 2x,1/4 \\
\quad (2,0,0,1/2) \ & \ (2,0,0,1/2)
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(4) x,y,z+1/2 [u,v,w]</td>
<td>(5) y,x+y,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) x-y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td>(11) x+y,y,z+1/2 [u+v,v,w]</td>
</tr>
<tr>
<td>6 h .2</td>
<td>x,2x,1/4 [u,2u,0]</td>
</tr>
<tr>
<td></td>
<td>x,2x,3/4 [u,2u,0]</td>
</tr>
<tr>
<td>6 g .2</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [u,0,0]</td>
</tr>
<tr>
<td>4 f 3..</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>4 e 3..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 d 3.2</td>
<td>1/3,2/3,3/4 [0,0,0]</td>
</tr>
<tr>
<td>2 c 3.2</td>
<td>1/3,2/3,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2 b 3.2</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2 a 3.2</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6m'm' Along [1,0,0] p2m'g' Along [2,1,0] p2m'g'

\begin{align*}
a^* &= a \\ b^* &= b \\
a^* &= c \\ b^* &= (a + 2b)/2 \\
a^* &= c \\ b^* &= b/2
\end{align*}

Origin at 0,0,0 Origin at x,0,0 Origin at x,x/2,1/4
Origin at 3211' at 6_3211'

Asymmetric unit

\[0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x < (1+y)/2; \quad y < \min(1-x,(1+x)/2)\]

Vertices

\[
\begin{align*}
 & 0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/3,3/4,0 & 0,1/2,0 \\
 & 0,0,1/4 & 1/2,0,1/4 & 2/3,1/3,1/4 & 1/3,3/4,1/4 & 0,1/2,1/4
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
 & (1) \ 1 \\
 & \quad (1|0,0,0) \\
 & (4) \ 2 \ (0,0,1/2) \ 0,0,z \\
 & \quad (2_z|0,0,1/2) \\
 & (7) \ 2 \ x,x,0 \\
 & \quad (2_x,0,0,0) \\
 & (10) \ 2 \ x,x,1/4 \\
 & \quad (2,0,0,1/2)
\end{align*}
\]

\[
\begin{align*}
 & (2) \ 3^+ \ 0,0,z \\
 & \quad (3_z|0,0,0) \\
 & (5) \ 6^* \ (0,0,1/2) \ 0,0,z \\
 & \quad (6_z^{-1}|0,0,1/2) \\
 & (8) \ 2 \ x,0,0 \\
 & \quad (2_x,0,0,0) \\
 & (11) \ 2 \ x,2x,1/4 \\
 & \quad (2_x,0,0,1/2)
\end{align*}
\]

\[
\begin{align*}
 & (3) \ 3^- \ 0,0,z \\
 & \quad (3_z^{-1}|0,0,0) \\
 & (6) \ 6^* \ (0,0,1/2) \ 0,0,z \\
 & \quad (6_z|0,0,1/2) \\
 & (9) \ 2 \ 0,y,0 \\
 & \quad (2_y,0,0,0) \\
 & (12) \ 2 \ 2x,x,1/4 \\
 & \quad (2_x,0,0,1/2)
\end{align*}
\]
Continued

For $1'$ set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
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<tbody>
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<td>$(1)$ $1'$</td>
<td>$x,y,z$ [0,0,0]</td>
</tr>
<tr>
<td>$(2)$ $3'$</td>
<td>$y,-x,-y,z$ [0,0,0]</td>
</tr>
<tr>
<td>$(3)$ $3'$</td>
<td>$x+y+xy, z$ [0,0,0]</td>
</tr>
<tr>
<td>$(4)$ $3'$</td>
<td>$x+y+xy,z+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$(5)$ $3'$</td>
<td>$x+y+xy, z+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$(6)$ $3'$</td>
<td>$x+y+xy, z+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$(7)$ $2'$</td>
<td>$x,2x,1/4$ [0,0,0]</td>
</tr>
<tr>
<td>$(8)$ $2'$</td>
<td>$2x_\perp, x_\perp, 1/4$ [0,0,0]</td>
</tr>
<tr>
<td>$(9)$ $2'$</td>
<td>$x+y, x+y, z$ [0,0,0]</td>
</tr>
<tr>
<td>$(10)$ $2'$</td>
<td>$y, x, z+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$(11)$ $2'$</td>
<td>$x, x, z+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$(12)$ $2'$</td>
<td>$x, x, z+1/2$ [0,0,0]</td>
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</tbody>
</table>

Generators selected

$(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'$.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i $11'$</td>
<td>$x,y,z$ [0,0,0]</td>
</tr>
<tr>
<td>6 h .21'</td>
<td>$x,2x,1/4$ [0,0,0]</td>
</tr>
<tr>
<td>6 g .21'</td>
<td>$x,0,0$ [0,0,0]</td>
</tr>
<tr>
<td>4 f $3.1'$</td>
<td>$1/3,2/3,z$ [0,0,0]</td>
</tr>
<tr>
<td>4 e $3.1'$</td>
<td>$0,0,z$ [0,0,0]</td>
</tr>
<tr>
<td>2 d $3.21'$</td>
<td>$1/3,2/3,3/4$ [0,0,0]</td>
</tr>
<tr>
<td>2 c $3.21'$</td>
<td>$1/3,2/3,1/4$ [0,0,0]</td>
</tr>
<tr>
<td>2 b $3.21'$</td>
<td>$0,0,1/4$ [0,0,0]</td>
</tr>
<tr>
<td>2 a $32.1'$</td>
<td>$0,0,0$ [0,0,0]</td>
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</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p6mm1’
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p2mg1’
\[ a^* = c \quad b^* = (a + 2b)/2 \]
Origin at x,0,0

Along [2,1,0] p2mg1’
\[ a^* = c \quad b^* = b/2 \]
Origin at x,x/2,1/4
**Origin** at 32'1 at 6'2'1

**Asymmetric unit**

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \]

**Vertices**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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<tbody>
<tr>
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</table>

**Symmetry Operations**

1. \( 1 \)
2. \( 1^* \)
3. \( 3^* \)
4. \( 2' \) \((0,0,1/2)\)
5. \( 6' \) \((0,0,1/2)\)
6. \( 6' \) \((0,0,1/2)\)
7. \( 2' \) \(x,x,0\)
8. \( 2' \) \(x,0,0\)
9. \( 2' \) \(0,y,0\)
10. \( 2 \) \(x,x,1/4\)
11. \( 2 \) \(x,2x,1/4\)
12. \( 2 \) \(2x,x,1/4\)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
<td>(5) y,x+y,z+1/2 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) x-y,y,z [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(10) x,y,z+1/2 [v,u,w]</td>
<td>(11) x+y,y,z+1/2 [u+v,v,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6' mm'</th>
<th>Along [1,0,0]</th>
<th>p2'm'g</th>
<th>Along [2,1,0]</th>
<th>p2mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = c \ b* = (a + 2b)/2</td>
<td>a* = c</td>
<td>b* = b/2</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,0</td>
<td>Origin at 0,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,1/4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin at 321 at 6'_21

Asymmetric unit

\[0 \leq x \leq 2/3;\ \ 0 \leq y \leq 2/3;\ \ 0 \leq z \leq 1/4;\ \ x \leq (1+y)/2;\ \ y \leq \min(1-x,(1+x)/2)\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,1/4 & \quad 0,1/2,0 \\
0,0,1/4 & \quad 1/2,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/3,2/3,1/4 & \quad 0,1/2,1/4
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) 1 & \quad (2) 3^* 0,0,z & \quad (3) 3^{-1} 0,0,z \\
(1|0,0,0) & \quad (3_z|0,0,0) & \quad (3_z^{-1}|0,0,0) \\
(4) 2' (0,0,1/2) & \quad 0,0,z & \quad (5) 6' - (0,0,1/2) & \quad 0,0,z & \quad (6) 6' - (0,0,1/2) & \quad 0,0,z \\
(2_z|0,0,1/2)' & \quad (6_z^{-1}|0,0,1/2)' & \quad (6_z|0,0,1/2)' \\
(7) 2 x,x,0 & \quad (8) 2 x,0,0 & \quad (9) 2 0,y,0 \\
(2_x|0,0,0) & \quad (2|0,0,0) & \quad (2_y|0,0,0) \\
(10) 2' x,x,1/4 & \quad (11) 2' x,2x,1/4 & \quad (12) 2' 2x,x,1/4 \\
(2_z|0,0,1/2)' & \quad (2_z|0,0,1/2)' & \quad (2|0,0,1/2)' \\
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(2) ( \bar{y},x-y,z ) [(v),u-v,w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(3) ( x+y,\bar{x},z ) [(u)+v,(\bar{u}),w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(4) ( \bar{x},y,z+1/2 ) [u,v,w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(5) ( y,x+y,z+1/2 ) [v,u-v,w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(6) ( x-y,x,z+1/2 ) [u+v,(\bar{u}),w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(7) ( \bar{y},x,z ) [v,u,w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(8) ( x-y,\bar{y},z ) [u-v,(\bar{v}),w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(9) ( \bar{x},x+y,z ) [(\bar{u}),u+v,w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(10) ( \bar{y},x,z+1/2 ) [v,u,w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(11) ( x-y,y,z+1/2 ) [u-v,(\bar{v}),w]</td>
</tr>
<tr>
<td>12 i 1</td>
<td>(12) ( \bar{x},x-y,z+1/2 ) [u,(\bar{u})+v,w]</td>
</tr>
</tbody>
</table>

6 h \( .2' \)  
\( x,2x,1/4 \) [u,0,w]  
\( 2x,\bar{x},1/4 \) [0,u,w]  
\( x,\bar{x},1/4 \) [\(\bar{u}\),\(\bar{u}\),w]  

6 g \( .2 \)  
\( x,0,0 \) [u,0,0]  
\( 0,x,0 \) [0,u,0]  
\( x,0,0 \) [\(\bar{u}\),0,0]  

4 f \( .3 . \)  
\( 1/3,2/3,z \) [0,0,w]  
\( 2/3,1/3,z+1/2 \) [0,0,w]  
\( 2/3,1/3,\bar{z} \) [0,0,w]  
\( 1/3,2/3,\bar{z}+1/2 \) [0,0,w]  

4 e \( .3 . \)  
\( 0,0,z \) [0,0,w]  
\( 0,z+1/2 \) [0,0,w]  
\( 0,0,z \) [0,0,w]  
\( 0,0,\bar{z}+1/2 \) [0,0,w]  

2 d \( 3.2' \)  
\( 1/3,2/3,3/4 \) [0,0,w]  
\( 2/3,1/3,1/4 \) [0,0,w]  

2 c \( 3.2' \)  
\( 1/3,2/3,1/4 \) [0,0,w]  
\( 2/3,1/3,3/4 \) [0,0,w]  

2 b \( 3.2' \)  
\( 0,0,1/4 \) [0,0,w]  
\( 0,0,3/4 \) [0,0,w]  

2 a \( 32. \)  
\( 0,0,0 \) [0,0,0]  
\( 0,0,1/2 \) [0,0,0]  

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a )</td>
<td>( b^* = b )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = c )</td>
<td>( b^* = (a + 2b)/2 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p2'm'g</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = c )</td>
<td>( b^* = b/2 )</td>
</tr>
</tbody>
</table>

Origin at 0,0,z  
Origin at 0,0,0  
Origin at x/2,1/4
Origin at 32'1 at 62'2'

Asymmetric unit:

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{4}; \quad x \leq (1+y)/2; \quad y \leq \min(1-x, (1+x)/2)\]

Vertices:

\[
\begin{align*}
0,0,0 & \quad \frac{1}{2},0,0 & \quad \frac{2}{3},\frac{1}{3},0 & \quad \frac{1}{3},\frac{2}{3},0 & \quad 0,\frac{1}{2},0 \\
0,0,\frac{1}{4} & \quad \frac{1}{2},0,\frac{1}{4} & \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} & \quad \frac{1}{3},\frac{2}{3},\frac{1}{4} & \quad 0,\frac{1}{2},\frac{1}{4}
\end{align*}
\]

Symmetry Operations:

1. \(1\)
2. \(3^* \ 0,0,z \quad (3z) \ 0,0,z\)
3. \(3^* \ 0,0,z \quad (3z^{-1}) \ 0,0,z\)
4. \(2 \ (0,0,1/2) \ 0,0,z \quad (2z) \ 0,0,1/2\)
5. \(6^* \ (0,0,1/2) \ 0,0,z \quad (6_{z^{-1}}) \ 0,0,1/2\)
6. \(6^* \ (0,0,1/2) \ 0,0,z \quad (6_{0,0,1/2})\)
7. \(2' \ x,x,0 \quad (2_{xy}) \ 0,0,0\)'
8. \(2' \ x,0,0 \quad (2_{z}) \ 0,0,0\)'
9. \(2' \ 0,y,0 \quad (2_{y}) \ 0,0,0\)'
10. \(2' \ x,x,1/4 \quad (2_{z}) \ 0,0,1/2\)'
11. \(2' \ x,2x,1/4 \quad (2_{z}) \ 0,0,1/2\)'
12. \(2' \ 2x,x,1/4 \quad (2_{z}) \ 0,0,1/2\)'

182.5.1414 - 1 - 3080
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [v,w]</td>
<td>(5) y,x+y,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,w]</td>
<td>(8) x-y,x,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/2 [v,w]</td>
<td>(11) x+y,x,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td>6 h .2'</td>
<td>x,2x,1/4 [u,0,w]</td>
<td>2x,x,1/4 [0,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,2x,3/4 [u,0,w]</td>
<td>2x,x,3/4 [0,u,w]</td>
</tr>
<tr>
<td>6 g .2'</td>
<td>x,0,0 [u,2u,w]</td>
<td>0,x,0 [2u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
</tr>
<tr>
<td>4 f 3..</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4 e 3..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2 d 3.2'</td>
<td>1/3,2/3,3/4 [0,0,w]</td>
<td>2/3,1/3,1/4 [0,0,w]</td>
</tr>
<tr>
<td>2 c 3.2'</td>
<td>1/3,2/3,1/4 [0,0,w]</td>
<td>2/3,1/3,3/4 [0,0,w]</td>
</tr>
<tr>
<td>2 b 3.2'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
</tr>
<tr>
<td>2 a 32'.</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

- Along [0,0,1] p6mm
  - a = a  b = b
  - Origin at 0,0,0
- Along [1,0,0] p2'mg'
  - a' = c  b' = (a + 2b)/2
  - Origin at 0,0,0
- Along [2,1,0] p2'mg'
  - a' = c  b' = b/2
  - Origin at x/2,1/4

182.5.1414 - 2 - 3081
**Origin** on 6mm

**Asymmetric unit**

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2 \]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^* \quad 0,0,z \\
(3) & \quad 0,0,0 \\
(4) & \quad 2 \quad 0,0,z \\
(5) & \quad 2 \quad 0,0,0 \\
(5) & \quad 0,0,z \\
(6) & \quad 0,0,0 \\
(6) & \quad 0,0,0 \\
(7) & \quad m \quad x,x,z \\
(7) & \quad m \quad x,x,0 \\
(7) & \quad m \quad x,0,z \\
(8) & \quad m \quad x,x,z \\
(8) & \quad m \quad x,x,0 \\
(8) & \quad m \quad x,0,z \\
(9) & \quad m \quad 2x,x,z \\
(9) & \quad m \quad 2x,x,0 \\
(9) & \quad m \quad 2x,0,z \\
(10) & \quad m \quad x,x,z \\
(10) & \quad m \quad x,x,0 \\
(10) & \quad m \quad x,0,z \\
(11) & \quad m \quad x,0,z \\
(11) & \quad m \quad x,0,0 \\
(11) & \quad m \quad x,0,0 \\
(12) & \quad m \quad 0,y,z \\
(12) & \quad m \quad 0,y,0 \\
(12) & \quad m \quad 0,y,0
\end{align*}
\]
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coords</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>12 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y,x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) x+y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td>(10) y,x,z [v,u,w]</td>
<td>(11) x-y,y,z [v,u+v,v,w]</td>
</tr>
<tr>
<td>6 e .m.</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>x,x,z [u,u,0]</td>
<td>x,2x,z [u,0,0]</td>
</tr>
<tr>
<td>6 d ..m</td>
<td>x,0,z [u,2u,0]</td>
</tr>
<tr>
<td>x,0,z [u,2u,0]</td>
<td>0,x,z [2u,u,0]</td>
</tr>
<tr>
<td>3 c 2mm</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 b 3m</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>1 a 6mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6mm
\( a^* = a \quad b^* = b \)
Origin at 0,0,z

Along [1,0,0] p1m11'
\( a^* = (a + 2b)/2 \quad b^* = c \)
Origin at x,0,0

Along [2,1,0] p1m11'
\( a^* = b/2 \quad b^* = c \)
Origin at x,x/2,0
Origin on 6mm1'

Asymmetric unit

\[ 0 \leq x < \frac{2}{3}; \quad 0 \leq y < \frac{1}{3}; \quad 0 \leq z < 1; \quad x < \frac{(1+y)}{2}; \quad y < \frac{x}{2} \]

Vertices

\[
\begin{align*}
0,0,0 & \quad \frac{1}{2},0,0 & \quad \frac{2}{3},\frac{1}{3},0 \\
0,0,1 & \quad \frac{1}{2},0,1 & \quad \frac{2}{3},\frac{1}{3},1
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \ 1 \quad (1) \ & 1 \quad (1) \ & 1 \\
& \ (1|0,0,0) & \ (1|0,0,0) & \ (1|0,0,0) \\
(2) & \ 3^+ \ 0,0,z \quad (2) & \ 3^+ \ 0,0,z \quad (2) & \ 3^+ \ 0,0,z \\
& \ (3z_1|0,0,0) & \ (3z_1|0,0,0) & \ (3z_1|0,0,0) \\
(4) & \ 2 \ 0,0,z \quad (4) & \ 2 \ 0,0,z \quad (4) & \ 2 \ 0,0,z \\
& \ (2z_1|0,0,0) & \ (2z_1|0,0,0) & \ (2z_1|0,0,0) \\
(5) & \ 6^- \ 0,0,z \quad (5) & \ 6^- \ 0,0,z \quad (5) & \ 6^- \ 0,0,z \\
& \ (6z_1^{-1}|0,0,0) & \ (6z_1^{-1}|0,0,0) & \ (6z_1^{-1}|0,0,0) \\
(6) & \ 6^- \ 0,0,z \quad (6) & \ 6^- \ 0,0,z \quad (6) & \ 6^- \ 0,0,z \\
& \ (6z_1|0,0,0) & \ (6z_1|0,0,0) & \ (6z_1|0,0,0) \\
(7) & \ m \ x,x,z \quad (7) & \ m \ x,x,z \quad (7) & \ m \ x,x,z \\
& \ (m_{xy}|0,0,0) & \ (m_{xy}|0,0,0) & \ (m_{xy}|0,0,0) \\
(8) & \ m \ x,2x,z \quad (8) & \ m \ x,2x,z \quad (8) & \ m \ x,2x,z \\
& \ (m_{x}|0,0,0) & \ (m_{x}|0,0,0) & \ (m_{x}|0,0,0) \\
(9) & \ m \ 2x,x,z \quad (9) & \ m \ 2x,x,z \quad (9) & \ m \ 2x,x,z \\
& \ (m_{y}|0,0,0) & \ (m_{y}|0,0,0) & \ (m_{y}|0,0,0) \\
(10) & \ m \ x,x,z \quad (10) & \ m \ x,x,z \quad (10) & \ m \ x,x,z \\
& \ (m_{3}|0,0,0) & \ (m_{3}|0,0,0) & \ (m_{3}|0,0,0) \\
(11) & \ m \ x,0,z \quad (11) & \ m \ x,0,z \quad (11) & \ m \ x,0,z \\
& \ (m_{2}|0,0,0) & \ (m_{2}|0,0,0) & \ (m_{2}|0,0,0) \\
(12) & \ m \ 0,y,z \quad (12) & \ m \ 0,y,z \quad (12) & \ m \ 0,y,z \\
& \ (m_{1}|0,0,0) & \ (m_{1}|0,0,0) & \ (m_{1}|0,0,0)
\end{align*}
\]
For 1' + set

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Position</th>
<th>Multiplicity</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1'</td>
<td>x,y,z</td>
<td>12</td>
<td>f</td>
<td>x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>y-x,y,z</td>
<td>(2)</td>
<td>g</td>
<td>y-x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>x+y,z,x</td>
<td>(3)</td>
<td>h</td>
<td>x+y,z,x [0,0,0]</td>
</tr>
<tr>
<td>(4) 2'</td>
<td>x,y,z</td>
<td>(4)</td>
<td>i</td>
<td>x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(5) 6'</td>
<td>y,x+y,z</td>
<td>(5)</td>
<td>j</td>
<td>y,x+y,z [0,0,0]</td>
</tr>
<tr>
<td>(6) 6'</td>
<td>x+y,y,z</td>
<td>(6)</td>
<td>k</td>
<td>x+y,y,z [0,0,0]</td>
</tr>
<tr>
<td>(7) m'</td>
<td>x,x,z</td>
<td>(7)</td>
<td>l</td>
<td>x,x,z [0,0,0]</td>
</tr>
<tr>
<td>(m)</td>
<td>x,x,z</td>
<td>(8)</td>
<td>m</td>
<td>x,x,z [0,0,0]</td>
</tr>
<tr>
<td>(9)</td>
<td>x,x-z</td>
<td>(9)</td>
<td>n</td>
<td>x,x-z [0,0,0]</td>
</tr>
<tr>
<td>(10)</td>
<td>m',0,z</td>
<td>(10)</td>
<td>o</td>
<td>m',0,z [0,0,0]</td>
</tr>
<tr>
<td>(11)</td>
<td>m',0,z</td>
<td>(11)</td>
<td>p</td>
<td>m',0,z [0,0,0]</td>
</tr>
<tr>
<td>(12)</td>
<td>m',0,z</td>
<td>(12)</td>
<td>q</td>
<td>m',0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.
**Origin** on 6'M'm

**Asymmetric unit**

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq 1; \quad x \leq \frac{1+y}{2}; \quad y \leq \frac{x}{2}\]

**Vertices**

- \(0,0,0\)
- \(1/2,0,0\)
- \(2/3,1/3,0\)
- \(0,0,1\)
- \(1/2,0,1\)
- \(2/3,1/3,1\)

**Symmetry Operations**

1. \(1\)
2. \(3^* 0,0,z\)
   - \((3_z|0,0,0)\)
3. \(3' 0,0,z\)
   - \((3_z^{-1}|0,0,0)\)
4. \(2' 0,0,z\)
   - \((2_z|0,0,0)'\)
5. \(6^* 0,0,z\)
   - \((6_{-1}|0,0,0)'\)
6. \(6' 0,0,z\)
   - \((6_z|0,0,0)'\)
7. \(m' x,x,z\)
   - \((m_x|0,0,0)'\)
8. \(m' x,2x,z\)
   - \((m_x|0,0,0)'\)
9. \(m' 2x,x,z\)
   - \((m_y|0,0,0)'\)
10. \(m x,x,z\)
    - \((m|0,0,0)\)
11. \(m x,0,z\)
    - \((m_2|0,0,0)\)
12. \(m 0,y,z\)
    - \((m_1|0,0,0)\)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 f</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y,x,z [v,u,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p6m'm'</td>
</tr>
<tr>
<td>a* = a b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [2,1,0] p1m11'</td>
</tr>
<tr>
<td>a* = b/2 b* = c</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
**Origin** on $6'mm'$

**Asymmetric unit**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0 \leq x \leq 2/3$</td>
<td>$0 \leq y \leq 1/3$</td>
<td>$0 \leq z \leq 1$</td>
</tr>
<tr>
<td>$x \leq (1+y)/2$</td>
<td>$y \leq x/2$</td>
<td></td>
</tr>
</tbody>
</table>

**Vertices**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
</tr>
<tr>
<td>0,0,1</td>
<td>1/2,0,1</td>
<td>2/3,1/3,1</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. $1$
   
2. $3^*$ $0,0,z$
   $(3z_x|0,0,0)$
3. $3^*$ $0,0,z$
   $(3z_x^{-1}|0,0,0)$
4. $2' 0,0,z$
   $(2z_x|0,0,0)'$
5. $6' 0,0,z$
   $(6z_x^{-1}|0,0,0)'$
6. $6' 0,0,z$
   $(6z_x|0,0,0)'$
7. $m$ $x,x,z$
   $(m_{xy}|0,0,0)$
8. $m$ $x,2x,z$
   $(m_{xz}|0,0,0)$
9. $m$ $2x,x,z$
   $(m_{y}|0,0,0)$
10. $m'$ $x,x,z$
    $(m_{xy}'|0,0,0)$
11. $m'$ $x,0,z$
    $(m_{z}|0,0,0)'$
12. $m'$ $0,y,z$
    $(m_{y}|0,0,0)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 12 f 1 | (1) x,y,z [u,v,w]  
(2) y,x-y,z [v,u-v,w]  
(3) x+y,x,z [u+v,u,w]  
(4) x,y,z [u,v,w]  
(5) y,x+y,z [v,u-v,w]  
(6) x-y,x,z [u+v,u,w]  
(7) y,x,z [v,u,w]  
(8) x+y,y,z [u-v,v,w]  
(9) x,x-y,z [u,u+v,w]  
(10) y,x,z [v,u,w]  
(11) x-y,y,z [v,u-v,w]  
(12) x,x+y,z [u,u+v,w] |
| 6 e .m. | x,x,z [u,u,0]  
(2) x,2x,z [u,0,0]  
2x,x,z [0,u,0] |
| 6 d ..m' | x,0,z [u,0,w]  
0,x,z [0,u,w]  
2x,x,z [0,u,0] |
| 3 c 2'mm' | 1/2,0,z [u,0,0]  
0,1/2,z [0,u,0]  
1/2,1/2,z [u,u,0] |
| 2 b 3m. | 1/3,2/3,z [0,0,0]  
2/3,1/3,z [0,0,0] |
| 1 a 6'mm' | 0,0,z [0,0,0] |

### Symmetry of Special Projections

- **Along [0,0,1] p6'mm'**
  - Origin at 0,0,z
  - $a^* = a$  
  - $b^* = b$

- **Along [1,0,0] p1m1**
  - Origin at x,0,0
  - $a^* = (a + 2b)/2$  
  - $b^* = c$

- **Along [2,1,0] p1m1**
  - Origin at x,x/2,0
  - $a^* = b/2$  
  - $b^* = c$
Origin on $6m'm'$

**Asymmetric unit**

$0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2$

**Vertices**

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>2/3,1/3,0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0,0,1</td>
<td>1/2,0,1</td>
<td>2/3,1/3,1</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. $1$
   
   $(1|0,0,0)$

2. $3^+$ 0,0,z
   
   $(3_z|0,0,0)$

3. $3^-$ 0,0,z
   
   $(3_z^{-1}|0,0,0)$

4. $2^* 0,0,0$
   
   $(2_z|0,0,0)$

5. $6^* 0,0,0$
   
   $(6_z|0,0,0)$

6. $6^* 0,0,0$
   
   $(6_z|0,0,0)$

7. $m'/x,x,z$
   
   $(m_{xy}|0,0,0)'$

8. $m'/x,2x,z$
   
   $(m_x|0,0,0)'$

9. $m'/2x,x,z$
   
   $(m_y|0,0,0)'$

10. $m'/x,x,z$
    
    $(m_{3y}|0,0,0)'$

11. $m'/x,0,z$
    
    $(m_3|0,0,0)'$

12. $m'/0,y,z$
    
    $(m_1|0,0,0)'$
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 f 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>6 e m'</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>6 d m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td>3 c 2m'</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td>2 b 3m'</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>1 a 6m’</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6m'm'</th>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
<th>Along [2,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (a + 2b)/2</td>
<td>b* = c</td>
<td>a* = b/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 6mm

Asymmetric unit  
0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/3; 0 ≤ z ≤ 1; x ≤ (1+y)/2; y ≤ x/2

Vertices  
0,0,0 1/2,0,0 2/3,1/3,0 0,0,1 1/2,0,1 2/3,1/3,1

Symmetry Operations  
For (0,0,0) + set

(1) 1  
(1|0,0,0)

(2) 3⁺ 0,0,z  
(3z|0,0,0)

(3) 3⁻ 0,0,z  
(3⁻|0,0,0)

(4) 2,0,0,z  
(2z|0,0,0)

(5) 6⁻ 0,0,z  
(6⁻|0,0,0)

(6) 6⁺ 0,0,z  
(6⁺|0,0,0)

(7) m x,x,z  
(mₓ|0,0,0)

(8) m x,2x,z  
(mₓ|0,0,0)

(9) m 2x,x,z  
(mᵧ|0,0,0)

(10) m x,x,z  
(mₓ|0,0,0)

(11) m x,0,z  
(mₓ|0,0,0)

(12) m 0,y,z  
(mᵧ|0,0,0)
For \((0,0,1)' + \) set

\(1\) \(t'(0,0,1)\) \(1\) \(0,0,1)' \(2\) \(3'(0,0,1)\) \(0,0,z\) \(3\) \(3'(0,0,1)\) \(0,0,z\) 

\(2\) \(2'(0,0,1)\) \(0,0,z\) \(5\) \(6'(0,0,1)\) \(0,0,z\) \(6\) \(6'(0,0,1)\) \(0,0,z\) 

\(7\) \(c'(0,0,1)\) \(x,x,z\) \(m_x|0,0,1)' \(8\) \(c'(0,0,1)\) \(x,2x,z\) \(m_x|0,0,1)' \(9\) \(c'(0,0,1)\) \(2x,x,z\) \(m_y|0,0,1)' 

\(10\) \(c'(0,0,1)\) \(x,x,z\) \(m_y|0,0,1)' \(11\) \(c'(0,0,1)\) \(x,0,z\) \(m_z|0,0,1)' \(12\) \(c'(0,0,1)\) \(0,y,z\) \(m_z|0,0,1)' 

Generators selected \(1; t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).\)

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

| Multiplicity | Coordinates | \(\begin{array}{ccc}
\text{Wyckoff letter} & \text{Site Symmetry} \\
\end{array}\) |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>24 (f) (1)</td>
<td>(1) (x,y,z) [(u,v,w)]</td>
<td>(2) (y, x-y,z) [(v,u-w)]</td>
</tr>
<tr>
<td>(4) (x, y, z) [(u, v, w)]</td>
<td>(5) (y, x+y, z) ([v, u+v, w])</td>
<td>(6) (x-y, x, z) ([u-v, u, w])</td>
</tr>
<tr>
<td>(7) (y, x, z) ([v, u, w])</td>
<td>(8) (x+y, y, z) ([u-v, v, w])</td>
<td>(9) (x, x-y, z) ([u, u+v, w])</td>
</tr>
<tr>
<td>(10) (y, x, z) ([v, u, w])</td>
<td>(11) (x-y, y, z) ([u+v, v, w])</td>
<td>(12) (x, x+y, z) ([u, u-v, w])</td>
</tr>
<tr>
<td>12 (e) (m)</td>
<td>(x, x, z) ([u, u, 0])</td>
<td>(x, 2x, z) ([u, 0, 0])</td>
</tr>
<tr>
<td>(x, x, z) ([u, u, 0])</td>
<td>(x, 2x, z) ([u, 0, 0])</td>
<td>(2x, x, z) ([0, u, 0])</td>
</tr>
<tr>
<td>12 (d) (m)</td>
<td>(x, 0, z) ([u, 2u, 0])</td>
<td>(0, x, z) ([2u, u, 0])</td>
</tr>
<tr>
<td>(x, 0, z) ([u, 2u, 0])</td>
<td>(0, x, z) ([2u, u, 0])</td>
<td>(x, x, z) ([u, u, 0])</td>
</tr>
<tr>
<td>(6) (c)</td>
<td>(2mm)</td>
<td>(1/2, 0, z) ([0, 0, 0])</td>
</tr>
<tr>
<td>4 (b)</td>
<td>(3m)</td>
<td>(1/3, 2/3, z) ([0, 0, 0])</td>
</tr>
<tr>
<td>2 (a)</td>
<td>(6mm)</td>
<td>(0, 0, z) ([0, 0, 0])</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

\(\begin{array}{ccc}
\text{Along} [0,0,1] & \text{p6mm} & \text{Along} [1,0,0] & \text{p1m11}' \\\n\text{Along} [2,1,0] & \text{p1m11}' \\\n\end{array}\)

\(\begin{array}{ccc}
\text{a}^* = \text{a} & \text{b}^* = \text{b} & \text{a}^* = (\text{a} + 2\text{b})/2 & \text{b}^* = \text{c} \\\n\text{Origin at 0,0,z} & \text{Origin at x,0,0} & \text{Origin at x,2,0} \\\n\end{array}\)
Origin on 6'm'm

Asymmetric unit  
0 ≤ x ≤ 2/3;  0 ≤ y ≤ 1/3;  0 ≤ z ≤ 1;  x ≤ (1+y)/2;  y ≤ x/2

Vertices  
0,0,0 1/2,0,0 2/3,1/3,0 0,0,1 1/2,0,1 2/3,1/3,1

Symmetry Operations

For (0,0,0) + set

1  
(1 0,0,0)  

(2) 3* 0,0,z  
(3) 3^-1 0,0,z  

(4) 2' 0,0,z  
(2,0,0)'  

(5) 6' 0,0,z  
(6) 6' - 0,0,z  

(7) m' x,x,z  
(m_y 0,0,0)'  

(8) m' x,2x,z  
(m_y 0,0,0)'  

(9) m' 2x,x,z  
(m_y 0,0,0)'  

(10) m x,x,z  
(m_3 0,0,0)  

(11) m x,0,z  
(m_2 0,0,0)  

(12) m 0,y,z  
(m_1 0,0,0)
Continued

(1) t' (0,0,1)
(2) 3' (0,0,1) 0,0,z
(3) 3' (0,0,1) 0,0,z
(4) 2 (0,0,1) 0,0,z
(5) 6 (0,0,1) 0,0,z
(6) 6' (0,0,1) 0,0,z
(7) c (0,0,1) x,x,z
(8) c (0,0,1) x,2x,z
(9) c (0,0,1) 2x,x,z
(10) c' (0,0,1) x,x,z
(11) c' (0,0,1) x,0,z
(12) c' (0,0,1) 0,y,z

Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

 Coordinates
(0,0,0) + (0,0,1)' +

24 f 1 (1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w]
(4) x,y,z [u,v,w] (5) x+y,z [v,u-v,w] (6) x-y,x,z [u+v,u,w]
(7) y,x,z [v,u,w] (8) x+y,y,z [u+v,v,w] (9) x-x,y,z [u,u-v,w]
(10) y,x,z [v,u,w] (11) x-y,y,z [u+v,v,w] (12) x-y+x,y,z [u,u-v,w]

12 e.m'. x,x,z [u,u,w] x,2x,z [u,2u,w]
(13) x,x,z [u,u,w] (14) x,2x,z [u,2u,w] 2x,x,z [2u,u,w]

12 d.m x,0,z [u,2u,0] 0,x,z [2u,u,0]
(15) x,0,z [u,2u,0] (16) 0,x,z [2u,u,0] x,x,z [u,u,0]

6 c 2'm'm 1/2,0,z [u,2u,0] 0,1/2,z [2u,u,0]
(17) 1/2,0,z [u,2u,0] (18) 0,1/2,z [2u,u,0] 1/2,1/2,z [u,u,0]

4 b 3'm' 1/3,2/3,z [0,0,w] 2/3,1/3,z [0,0,w]
(19) 1/3,2/3,z [0,0,w] (20) 2/3,1/3,z [0,0,w]

2 a 6'm'm 0,0,z [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p6mm1' Along [1,0,0] p2mm1 Along [2,1,0] p1m11'
a* = a b* = b a* = (a + 2b)/2 b* = c a* = b/2 b* = c
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0

183.7.1421 - 2 - 3095
**Origin** on 6\(\text{mm}'\)

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2
\]

**Vertices**

\[
(0,0,0) \quad 1/2,0,0 \quad 2/3,1/3,0
0,0,1 \quad 1/2,0,1 \quad 2/3,1/3,1
\]

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

(1) \(1\)

(2) \(3^+ 0,0,z\)

(3) \(3^- 0,0,z\)

(4) \(2' 0,0,z\)

(5) \(6^- 0,0,z\)

(6) \(6^+ 0,0,z\)

(7) \(m x,x,z\)

(8) \(m x,2x,z\)

(9) \(m 2x,x,z\)

(10) \(m' x,x,z\)

(11) \(m' x,0,z\)

(12) \(m' 0,y,z\)
Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinate</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 f 1</td>
<td>(0,0,0) + (0,0,1)' +</td>
<td>x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
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<tr>
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<td>(3) x+y,x,z [u+v,u,w]</td>
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<td>(4) x,y,z [u,v,w]</td>
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<td>(5) y,x+y,z [v,u-v,w]</td>
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<td>(6) x-y,x,z [u+v,u,w]</td>
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<td>(7) y,x,z [v,u,w]</td>
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<td>(8) x+y,y,z [u-v,v,w]</td>
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<td>(9) x,x-y,z [u,u+v,w]</td>
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<td>(10) y,x,z [v,u,w]</td>
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<td></td>
<td></td>
<td>(11) x-y,y,z [v-u-v,w]</td>
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<td>(12) x,x+y,z [u+u+v,w]</td>
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<tr>
<td>12 e .m.</td>
<td>x,x,z [u,u,0]</td>
<td></td>
<td>x,x,z [u,u,0]</td>
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<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
<td></td>
<td>x,2x,z [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
<td></td>
<td>2x,x,z [0,u,0]</td>
</tr>
<tr>
<td>12 d .m'</td>
<td>x,0,z [u,0,w]</td>
<td></td>
<td>x,0,z [0,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,z [u,0,w]</td>
<td></td>
<td>x,0,z [0,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,z [u,0,w]</td>
<td></td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>6 c 2'mm'</td>
<td>1/2,0,z [u,0,0]</td>
<td></td>
<td>0,1/2,z [0,u,0]</td>
</tr>
<tr>
<td>4 b 3m.</td>
<td>1/3,2/3,z [0,0,0]</td>
<td></td>
<td>2/3,1/3,z [0,0,0]</td>
</tr>
<tr>
<td>2 a 6'mm'</td>
<td>0,0,z [0,0,0]</td>
<td></td>
<td>0,0,z [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>[0,0,1]</th>
<th>[1,0,0]</th>
<th>[2,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>a* = (a + 2b)/2</td>
<td>a* = b/2</td>
<td></td>
</tr>
<tr>
<td>b* = b</td>
<td>b* = c</td>
<td>b* = c</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>

183.8.1422 - 2 - 3097
P₂c 6mm' 6mm1' Hexagonal
183.9.1423 P₂c 6mm'

Origin on 6mm'

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2 \]

Vertices

\[ \begin{array}{ccc}
0,0,0 & 1/2,0,0 & 2/3,1/3,0 \\
0,0,1 & 1/2,0,1 & 2/3,1/3,1 \\
\end{array} \]

Symmetry Operations

For \((0,0,0) + \) set

\[ \begin{array}{ccc}
(1) 1 & (2) 3' 0,0,z & (3) 3' 0,0,z \\
(1) 0,0,0 & (3) 3' 0,0,0 & (3) 3' 0,0,0 \\
(4) 2 0,0,z (2z) 0,0,0 & (5) 6' 0,0,z (6z) 0,0,0 & (6) 6' 0,0,z (6z) 0,0,0 \\
(m' x,x,z) (m_y 0,0,0)' & (8) m' x,2x,z (m_x 0,0,0)' & (9) m' 2x,x,z (m_y 0,0,0)' \\
(m' x,x,z) (m_3 0,0,0)' & (11) m' x,0,z (m_2 0,0,0)' & (12) m' 0,y,z (m_1 0,0,0)' \\
\end{array} \]

183.9.1423 - 1 - 3098
Continued

(1) t' (0,0,1) (1) 0,0,1' (1) t' (0,0,1)
(2) 3 + (0,0,1) 0,0,z (2) 3 + (0,0,1) 0,0,z
(3) 3 + (0,0,1) 0,0,z (3) 3 + (0,0,1) 0,0,z
(4) 2 + (0,0,1) 0,0,z (4) 2 + (0,0,1) 0,0,z
(2) 0,0,1' (2) 0,0,1' (2) 0,0,1'
(5) 6 + (0,0,1) 0,0,z (5) 6 + (0,0,1) 0,0,z
(6) 6 + (0,0,1) 0,0,z (6) 6 + (0,0,1) 0,0,z
(7) c (0,0,1) x,x,z (7) c (0,0,1) x,x,z
(m,z) (0,0,1) (m,z) (0,0,1)
(8) c (0,0,1) x,2x,z (8) c (0,0,1) x,2x,z
(m,x) (0,0,1) (m,x) (0,0,1)
(9) c (0,0,1) 2x,x,z (9) c (0,0,1) 2x,x,z
(m,y) (0,0,1) (m,y) (0,0,1)
(10) c (0,0,1) x,x,z (10) c (0,0,1) x,x,z
(m,y) (0,0,1) (m,y) (0,0,1)
(11) c (0,0,1) x,0,z (11) c (0,0,1) x,0,z
(m,z) (0,0,1) (m,z) (0,0,1)
(12) c (0,0,1) 0,y,z (12) c (0,0,1) 0,y,z
(m,x) (0,0,1) (m,x) (0,0,1)

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 f 1</td>
<td>(0,0,0) + (0,0,1)' +</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,z [u+v,u,w]</td>
<td>(3) x+y,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z [v,u+v,w]</td>
<td>(5) y,x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z [u-v,u,w]</td>
<td>(6) x-y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+y,y,z [u+v,v,w]</td>
<td>(8) x+y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,y-z [u,u-v,w]</td>
<td>(9) x,y-z [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z [v,u,w]</td>
<td>(10) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x-y,z [u-v,u,w]</td>
<td>(11) x-y,z [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,x+y,z [u,u+v,w]</td>
<td>(12) x,x+y,z [u,u+v,w]</td>
</tr>
<tr>
<td>12 e .m'</td>
<td>x,x,z [u,u,w]</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,2x,z [u,2u,w]</td>
<td>x,2x,z [u,2u,w]</td>
</tr>
<tr>
<td></td>
<td>2x,x,z [2u,2u,w]</td>
<td>2x,x,z [2u,2u,w]</td>
</tr>
<tr>
<td>12 d .m'</td>
<td>x,0,z [u,0,w]</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,x,z [0,u,w]</td>
<td>0,x,z [0,u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,w]</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>6 c 2m'm'</td>
<td>1/2,0,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4 b 3m'</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>2 a 6m'm'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6mm1' Along [1,0,0] p21m'1 Along [2,1,0] p21m'1
a* = a b* = b a* = (a + 2b)/2 b* = c a* = b/2 b* = c
Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
**Origin** on 6cc

**Asymmetric unit**
- $0 \leq x \leq 2/3$;
- $0 \leq y \leq 1/2$;
- $0 \leq z \leq 1/2$;
- $x \leq (1+y)/2$;
- $y \leq \min(1-x,x)$

**Vertices**
- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/2,1/2,0$
- $0,0,1/2$
- $1/2,0,1/2$
- $2/3,1/3,1/2$
- $1/2,1/2,1/2$

**Symmetry Operations**

1. $1$
2. $3^* \, 0,0,z$
3. $3^* \, 0,0,z$
4. $2 \, 0,0,z$
5. $6^* \, 0,0,z$
6. $6^* \, 0,0,z$
7. $c \, (0,0,1/2) \ x,x,z$
8. $c \, (0,0,1/2) \ x,x,z$
9. $c \, (0,0,1/2) \ 2x,x,z$
10. $c \, (0,0,1/2) \ x,x,z$
11. $c \, (0,0,1/2) \ x,0,z$
12. $c \, (0,0,1/2) \ 0,y,z$

\[ \text{P6cc} \quad 6cc \quad \text{Hexagonal} \]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>12</th>
<th>d</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) y,x-y,z [v,u-v,w]</th>
<th>(3) x+y,x,z [u+v,u+w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y,x+y,z [v,u+v,w]</td>
<td>(6) x-y,x,z [u-v,u+w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>(8) x+y,y,z+1/2 [u-v,v,w]</td>
<td>(9) x,x-z+1/2 [u,u+v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td>(11) x-y,y,z+1/2 [u+v,v,w]</td>
<td>(12) x,x,y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>2..</td>
<td>1/2,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
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<tr>
<td></td>
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<td>0,1/2,z+1/2 [0,0,w]</td>
<td>1/2,0,z+1/2 [0,0,w]</td>
<td>1/2,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>3..</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>1/3,2/3,z+1/2 [0,0,w]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
<td>1/3,2/3,z+1/2 [0,0,w]</td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>6..</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6mm Along [1,0,0] p2b.1m'1 Along [2,1,0] p2b.1m'1

a* = a  b* = b  a* = (a + 2b)/2  b* = c/2
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
Origin on 6cc1'

Asymmetric unit

\[ \begin{align*}
0 \leq x \leq 2/3; & \quad 0 \leq y \leq 1/2; & \quad 0 \leq z \leq 1/2; & \quad x \leq (1+y)/2; & \quad y \leq \min(1-x,x)
\end{align*} \]

Vertices

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>2/3,1/3,0</th>
<th>1/2,1/2,0</th>
<th>1/2,1/2,1/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1,3,1/2</td>
<td>1/2,1/2,1/2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

For 1 + set

(1) 1
(1) 0,0,0
(2) 3* 0,0,z
(2) 3z 0,0,0
(3) 3* 0,0,z
(3) 3z 0,0,0
(4) 2 0,0,z
(4) 0,0,0
(5) 6* 0,0,z
(5) 6z 0,0,0
(6) 6* 0,0,z
(6) 6z 0,0,0
(7) c (0,0,1/2) x,x,z
(7) m_y 0,0,1/2
(8) c (0,0,1/2) x,2x,z
(8) m_x 0,0,1/2
(9) c (0,0,1/2) 2x,x,z
(9) m_y 0,0,1/2
(10) c (0,0,1/2) x,x,z
(10) m_y 0,0,1/2
(11) c (0,0,1/2) x,0,z
(11) m_z 0,0,1/2
(12) c (0,0,1/2) 0,y,z
(12) m_z 0,0,1/2

184.2.1425 - 1 - 3102
For 1' + set

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d 11'</td>
<td>1 + 1' +</td>
</tr>
<tr>
<td>6</td>
<td>c 2..1'</td>
<td>1/2,0,z [0,0,0] 0,1/2,z [0,0,0] 1/2,1/2,z [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b 3..1'</td>
<td>1/3,2/3,z [0,0,0] 2/3,1/3,z [0,0,0] 1/3,2/3,z+1/2 [0,0,0] 2/3,1/3,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 6..1'</td>
<td>0,0,z [0,0,0] 0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6mm1'  
Along [1,0,0] p1m11'  
Along [2,1,0] p1m11'  
\[ a^* = a \quad b^* = b \]  
\[ a^* = (a + 2b)/2 \quad b^* = c/2 \]  
\[ a^* = b/2 \quad b^* = c/2 \]  
Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x/2,0
**Origin** on 6*c’c

**Asymmetric unit**
- $0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x)$

**Vertices**
- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/2,1/2,0
- 0,0,1/2
- 1/2,0,1/2
- 2/3,1/3,1/2
- 1/2,1/2,1/2

**Symmetry Operations**

1. $1$
2. $3^* 0,0,z$
3. $3^- 0,0,z$
4. $2' 0,0,z$
5. $6^- 0,0,z$
6. $6^+ 0,0,z$
7. $c' (0,0,1/2) x,x,z$
8. $c' (0,0,1/2) x,2x,z$
9. $c' (0,0,1/2) 2x,x,z$
10. $c (0,0,1/2) x,x,z$
11. $c (0,0,1/2) x,0,z$
12. $c (0,0,1/2) 0,y,z$
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 d 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) y,x+y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>(8) x+y,y,z+1/2 [u+ν,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td>(11) x-y,y,z+1/2 [u+ν,ν,ν,w]</td>
</tr>
</tbody>
</table>

| 6 c 2′. | 1/2,0,z [u,v,0] | 0,1/2,z [ν,u-v,0] |
|         | 0,1/2,z+1/2 [ν,u,0] | 1/2,0,z+1/2 [u+ν,v,0] |

| 4 b 3.. | 1/3,2/3,z [0,0,w] | 2/3,1/3,z [0,0,w] |
|         | 1/3,2/3,z+1/2 [0,0,w] | 2/3,1/3,z+1/2 [0,0,ν,w] |

| 2 a 6′.. | 0,0,z [0,0,0] | 0,0,z+1/2 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p6′m'm
\(a^* = a\) \(b^* = b\)
Origin at 0,0,z

Along [1,0,0] p1m1
\(a^* = (a + 2b)/2\) \(b^* = c/2\)
Origin at x,0,0

Along [2,1,0] \(p_{2\nu}m1\)
\(a^* = b/2\) \(b^* = c/2\)
Origin at x,x/2,0
Origin on 6'cc'

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq 2/3; \\
0 \leq y & \leq 1/2; \\
0 \leq z & \leq 1/2; \\
x & \leq (1+y)/2; \\
y & \leq \min(1-x, x)
\end{align*}
\]

Vertices

\[
\begin{align*}
n \quad & 0,0,0 \\
& 1/2,0,0 \\
& 2/3,1/3,0 \\
& 2/3,1/3,1/2 \\
& 1/2,1/2,0 \\
& 1/2,1/2,1/2 \\
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) \quad & 1 \\
(2') \quad & 0,0,z \\
(3') \quad & 0,0,Z \\
(4') \quad & 0,0,z \\
(6') \quad & 0,0,z \\
(6) \quad & 0,0,z \\
(7) \quad & c(0,0,1/2) \quad x,x,z \\
(8) \quad & c(0,0,1/2) \quad x,2x,z \\
(9) \quad & c(0,0,1/2) \quad 2x,x,z \\
(10) \quad & c'(0,0,1/2) \quad x,x,z \\
(11) \quad & c'(0,0,1/2) \quad x,0,z \\
(12) \quad & c'(0,0,1/2) \quad 0,y,z
\end{align*}
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z [v,u-v,w] (3) x+y,x,z [u+v,u,w] (4) x,y,z [u+v,u,w] (5) y,x+y,z [v,u-v,w] (6) x-y,x,z [u+v,u,w] (7) y,x,z+1/2 [v,u,w] (8) x+y,y,z+1/2 [u-v,v,w] (9) x,x,y,z+1/2 [u,u+v,w] (10) y,x,z+1/2 [v,u,w] (11) x-y,y,z+1/2 [u-v,v,w] (12) x,x+y,z+1/2 [u,u+v,w]</td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>1/2,0,z [u,v,0] 0,1/2,z [v,u-v,0] 1/2,1/2,z [u+v,u,0] 0,1/2,z+1/2 [v,u,v,0] 1/2,0,z+1/2 [u-v,v,0] 1/2,1/2,z+1/2 [u,u+v,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>1/3,2/3,z [0,0,w] 2/3,1/3,z [0,0,w] 1/3,2/3,z+1/2 [0,0,w] 1/3,1/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,z [0,0,0] 0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6'mm'</th>
<th>Along [1,0,0]</th>
<th>p2b*1m1</th>
<th>Along [2,1,0]</th>
<th>p1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
<td>(a^* = (a + 2b)/2)</td>
<td>(b^* = c/2)</td>
<td>(a^* = b/2)</td>
<td>(b^* = c/2)</td>
</tr>
</tbody>
</table>

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
Origin on 6c'c'

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x) \]

Vertices

\[ 0,0,0 \]
\[ 1/2,0,0 \]
\[ 2/3,1/3,0 \]
\[ 1/2,1/2,0 \]
\[ 0,0,1/2 \]
\[ 1/2,0,1/2 \]
\[ 2/3,1/3,1/2 \]
\[ 1/2,1/2,1/2 \]

Symmetry Operations

(1) 1
(1*0,0,0)

(2) 3* 0,0,z
(3z,0,0,0)

(3) 3' 0,0,z
(3z,-1,0,0,0)

(4) 2 0,0,z
(2z,0,0,0)

(5) 6* 0,0,z
(6z,-1,0,0,0)

(6) 6' 0,0,z
(6z,0,0,0)

(7) c'(0,0,1/2) x,x,z
(m_y,0,0,1/2')

(8) c'(0,0,1/2) x,2x,z
(m_x,0,0,1/2')

(9) c'(0,0,1/2) 2x,x,z
(m_y,0,0,1/2')

(10) c'(0,0,1/2) x,x,z
(m_y,0,0,1/2')

(11) c'(0,0,1/2) x,0,z
(m_x,0,0,1/2')

(12) c'(0,0,1/2) 0,y,z
(m_t,0,0,1/2')
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d 1</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+y,y,z+1/2 [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x-y,y,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x-y,x,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,x-y,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td>6</td>
<td>c 2..</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,z [0,0,w]</td>
</tr>
<tr>
<td>4</td>
<td>b 3..</td>
</tr>
<tr>
<td></td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/3,2/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a 6..</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a + 2b)/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = b/2</td>
<td>b* = c/2</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 31m at 63 cm

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{1+y}{2}; \quad y \leq \min(1-x,x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 & \quad (2) & \quad 3^* & \quad 0,0,z & \quad (3) & \quad 3^* & \quad 0,0,z \\
(10) & \quad m & \quad x,z & \quad (m_3 & \quad 0,0,0) & \quad (3^* & \quad 0,0,z & \quad (m_3^- & \quad 0,0,0) \\
(4) & \quad 2 & \quad (0,0,1/2) & \quad 0,0,z & \quad (2_z & \quad 0,0,1/2) & \quad (5) & \quad 6^* & \quad (0,0,1/2) & \quad 0,0,z & \quad (6) & \quad 6^* & \quad (0,0,1/2) & \quad 0,0,z & \quad (6_z & \quad 0,0,1/2) \\
(7) & \quad c & \quad (0,0,1/2) & \quad x,0,z & \quad (m_{xy} & \quad 0,0,1/2) & \quad (8) & \quad c & \quad (0,0,1/2) & \quad x,2x,z & \quad (m_x & \quad 0,0,1/2) & \quad (9) & \quad c & \quad (0,0,1/2) & \quad 2x,x,z & \quad (m_y & \quad 0,0,1/2) \\
(11) & \quad m & \quad 0,0,z & \quad (m_2 & \quad 0,0,0) & \quad (12) & \quad m & \quad 0,y,z & \quad (m_1 & \quad 0,0,0)
\end{align*}
\]


**Generators selected**  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>
| 12 d 1       | (1) x,y,z [u,v,w]  
               | (2) y,x-y,z [v-u,v,w]  
               | (3) x+y,x,z [u+v,u,w] |
|              | (4) x,y,z+1/2 [u,v,w]  
               | (5) y,x+y,z+1/2 [v,u+v,w]  
               | (6) x-y,x,z+1/2 [u-v,u,w] |
| 6 c m       | (7) y,x,z+1/2 [v,u,w]  
               | (8) x+y,y,z+1/2 [u-v,v,w]  
               | (9) x,x-y,z+1/2 [v-u,v,w] |
|              | (10) y,x,z [v,u,w]  
               | (11) x-y,y,z [v+u,v,w]  
               | (12) x,x+y,z [u,u-v,w] |
| 4 b 3..     | x,0,z [u,2u,0]  
               | 0,x,z [2u,u,0]  
               | x,x,z [u,u,0] |
| 2 a 3..     | x,0,z+1/2 [u,2u,0]  
               | 0,x,z+1/2 [2u,u,0]  
               | x,x,z+1/2 [u,u,0] |

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm</th>
<th>Along [1,0,0]</th>
<th>pab, 1m1</th>
<th>Along [2,1,0]</th>
<th>p1g11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td></td>
<td>b* = b</td>
<td></td>
<td>a* = b/2</td>
<td>b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>

---

185.1.1429 - 2 - 3111
Origin on 31m1' at 63 cm1'

Asymmetric unit

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{1+y}{2}; \quad y \leq \min(1-x,x)\]

Vertices

0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/2,1/2,0

0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2 \quad 1/2,1/2,1/2

Symmetry Operations

For 1 + set

\begin{align*}
(1) \ &1 \\
(1|0,0,0) \\
(2) \ &3^* \ 0,0,z \\
(3z|0,0,0) \\
(3) \ &3^* \ 0,0,z \\
(3z^{-1}|0,0,0) \\
(4) \ &2 \ (0,0,1/2) \ 0,0,z \\
(2_1|0,0,1/2) \\
(5) \ &6 \ (0,0,1/2) \ 0,0,z \\
(6_2|0,0,1/2) \\
(6) \ &6^* \ (0,0,1/2) \ 0,0,z \\
(6_2|0,0,1/2) \\
(7) \ &c \ (0,0,1/2) \ x,x,z \\
(m_{xy}|0,0,1/2) \\
(8) \ &c \ (0,0,1/2) \ x,2x,z \\
(m_{x}|0,0,1/2) \\
(9) \ &c \ (0,0,1/2) \ 2x,x,z \\
(m_{y}|0,0,1/2) \\
(10) \ &m \ x,x,z \\
(m_3|0,0,0) \\
(11) \ &m \ x,0,z \\
(m_2|0,0,0) \\
(12) \ &m \ 0,y,z \\
(m_1|0,0,0) \\
\end{align*}
Continued

For 1' + set

(1) 1'
   (1) [0,0,0]
(2) 3' + 0,0,z
   (3) [0,0,0]
(3) 3' + 0,0,z
   (4) [0,0,0]

(4) 2'(0,0,1/2) 0,0,z
   (2,1/2 0,0,1/2)
(5) 6' (0,0,1/2) 0,0,z
   (6,1 0,0,1/2)
(6) 6' + (0,0,1/2) 0,0,z
   (6,1 0,0,1/2)

(7) c' (0,0,1/2) x,x,z
   (m,x |0,0,1/2)
(8) c' (0,0,1/2) x,2x,z
   (m,x |0,0,1/2)
(9) c' (0,0,1/2) 2x,x,z
   (m,y |0,0,1/2)

(10) m' x,x,z
    (m,y |0,0,0)
(11) m' x,0,z
    (m,y |0,0,0)
(12) m' 0,y,z
    (m,x |0,0,0)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

Multiplicity, Coordinates
Wyckoff letter, Multiplicity,
Site Symmetry. Coordinates

12 d 11'  (1) x,y,z [0,0,0]  (2) y,x-y,z [0,0,0]  (3) x+y,x,z [0,0,0]
(4) x,y,z+1/2 [0,0,0]
(5) x,y,z+1/2 [0,0,0]  (6) x,y,x,z+1/2 [0,0,0]
(7) x,y,z+1/2 [0,0,0]  (8) x+y,y,z+1/2 [0,0,0]  (9) x,y,x,z+1/2 [0,0,0]
(10) y,x,z [0,0,0]  (11) x,y,x,z [0,0,0]  (12) x,y,x,z [0,0,0]

6 c ..m1'  x,0,z [0,0,0]  0,x,z [0,0,0]  x,x,z [0,0,0]
   x,0,z+1/2 [0,0,0]  0,x,z+1/2 [0,0,0]  x,x,z+1/2 [0,0,0]

4 b 3..1'  1/3,2/3,z [0,0,0]  2/3,1,3,z+1/2 [0,0,0]  1/3,2/3,z+1/2 [0,0,0]  2/3,1,3,z [0,0,0]

2 a 3.m1'  0,0,z [0,0,0]  0,0,z+1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p6mm1'  Along [1,0,0] p1m11'  Along [2,1,0] p1g11'
\( a^* = a \quad b^* = b \)
\( a^* = (a + 2b)/2 \quad b^* = c/2 \)  \( a^* = b/2 \quad b^* = c \)
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0

185.2.1430 - 2 - 3113
Origin on 31m at $6'_3$ c'm

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1') & \quad 0,0,0 \\
(2) & \quad 3' \quad 0,0,z \\
(3) & \quad 3' \quad 0,0,z \\
(4) & \quad 2' \quad (0,0,1/2) \quad 0,0,z \\
(5) & \quad 6' \quad (0,0,1/2) \quad 0,0,z \\
(6) & \quad 6' \quad (0,0,1/2) \quad 0,0,z \\
(7) & \quad c' \quad (0,0,1/2) \quad x,z \\
(8) & \quad c' \quad (0,0,1/2) \quad x,2x,z \\
(9) & \quad c' \quad (0,0,1/2) \quad 2x,x,z \\
(10) & \quad m \quad x,x,z \\
(11) & \quad m \quad x,0,z \\
(12) & \quad m \quad 0,y,z
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 d 1</td>
<td>(1) (x,y,z [u,v,w])</td>
</tr>
<tr>
<td></td>
<td>(4) (\bar{x},y,z+1/2 [v,u,w])</td>
</tr>
<tr>
<td></td>
<td>(7) (\bar{y},x,z+1/2 [v,u,w])</td>
</tr>
<tr>
<td></td>
<td>(10) (y,x,z [v,u,w])</td>
</tr>
<tr>
<td>6 c ..m</td>
<td>(x,0,z [u,2u,0])</td>
</tr>
<tr>
<td></td>
<td>(\bar{x},0,z+1/2 [u,2u,0])</td>
</tr>
<tr>
<td>4 b 3..</td>
<td>1/3,2/3,(z [0,0,w])</td>
</tr>
<tr>
<td>2 a 3..</td>
<td>0,0,(z [0,0,0])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'm'm  
Along [1,0,0] p1m1  
Along [2,1,0] p1g11'

\(a^* = a\)  
\(b^* = b\)  
\(a^* = (a + 2b)/2\)  
\(b^* = c/2\)  
\(a^* = b/2\)  
\(b^* = c\)

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x/2,0
Origin on 31m' at 6' cm'

Asymmetric unit

<table>
<thead>
<tr>
<th>Vertices</th>
<th>0 ≤ x ≤ 2/3;</th>
<th>0 ≤ y ≤ 1/2;</th>
<th>0 ≤ z ≤ 1/2;</th>
<th>x ≤ (1+y)/2;</th>
<th>y ≤ min(1-x,x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
<td>1/2,1/2,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1/3,1/2</td>
<td>1/2,1/2,1/2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) 1
(1) 0,0,0

(2) 3* 0,0,z
(3) 3* 0,0,z
(3) 0,0,0

(4) 2' (0,0,1/2) 0,0,z
(2', 0,0,1/2)

(5) 6' (0,0,1/2) 0,0,z
(6) 6' (0,0,1/2) 0,0,z
(6) 0,0,1/2')

(6) 6' (0,0,1/2) 0,0,z
(6) 0,0,1/2')

(7) c (0,0,1/2) x,x,z
(mₙₓ) 0,0,1/2)

(8) c (0,0,1/2) x,x,z
(mₙₓ) 0,0,1/2)

(9) c (0,0,1/2) 2x,x,z
(mₙₙ) 0,0,1/2)

(10) m' x,x,z
(mₙₙ) 0,0,0

(11) m' x,0,z
(mₙₙ) 0,0,0

(12) m' 0,y,z
(mₙₙ) 0,0,0

185.4.1432 - 1 - 3116
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d 1</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td>(4) x,y,z+1/2 [u,v,w]</td>
<td>(5) y,x+y,z+1/2 [v,u-v,w]</td>
</tr>
<tr>
<td>(7) x+y,x,z+1/2 [v,u,w]</td>
<td>(8) x+y,y,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td>(10) y,x,z [v,u,w]</td>
<td>(11) x-y,y,z [u-v,v,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6</th>
<th>c</th>
<th>..m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,0,z [u,0,w]</td>
<td>0,x,z [0,u,w]</td>
<td>x,x,z [u,u,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>b</th>
<th>3..</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
<td>1/3,2/3,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2</th>
<th>a</th>
<th>3.m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>x,x,z+1/2 [u,u,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Alice [0,0,1] p6'mm'</th>
<th>Along [1,0,0] p2b* 1m'1</th>
<th>Along [2,1,0] p1g1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = (a + 2b)/2</td>
<td>a* = b/2 b* = c</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
**Origin** on 31m' at 63 c'm'

**Asymmetric unit**

\[
0 < x < \frac{2}{3}; \quad 0 < y < \frac{1}{2}; \quad 0 < z < \frac{1}{2}; \quad x < \frac{1+y}{2}; \quad y < \min(1-x, x)
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z & \quad (3) & \quad 3^* \quad 0,0,z \\
(4) & \quad 2 \quad (0,0,1/2) \quad 0,0,z & \quad (5) & \quad 6' \quad (0,0,1/2) \quad 0,0,z & \quad (6) & \quad 6' \quad (0,0,1/2) \quad 0,0,z \\
(7) & \quad c' \quad (0,0,1/2) \quad x,x,z & \quad (8) & \quad c' \quad (0,0,1/2) \quad x,2x,z & \quad (9) & \quad c' \quad (0,0,1/2) \quad 2x,x,z \\
(10) & \quad m' \quad x,x,z & \quad (11) & \quad m' \quad x,0,z & \quad (12) & \quad m' \quad 0,y,z
\end{align*}
\]

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,0 & \quad (3) & \quad 3^* \quad 0,0,0 \\
(4) & \quad 2 \quad (0,0,1/2) \quad 0,0,0 & \quad (5) & \quad 6' \quad (0,0,1/2) \quad 0,0,0 & \quad (6) & \quad 6' \quad (0,0,1/2) \quad 0,0,0 \\
(7) & \quad c' \quad (0,0,1/2) \quad m_{xy},0,1/2 & \quad (8) & \quad c' \quad (0,0,1/2) \quad m_{x},0,1/2 & \quad (9) & \quad c' \quad (0,0,1/2) \quad m_{y},0,1/2 \\
(10) & \quad m' \quad m_{3},0,0,0 & \quad (11) & \quad m' \quad m_{2},0,0,0 & \quad (12) & \quad m' \quad m_{1},0,0,0
\end{align*}
\]
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) y,x+y,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x-y,x,z+1/2 [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
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<tr>
<td></td>
<td></td>
<td>(8) x+y,y,z+1/2 [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(9) x,x-y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(11) x-y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) x,y,z [u+v,u+v,w]</td>
</tr>
<tr>
<td>6</td>
<td>c ..m'</td>
<td>x,0,z [u,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,x,z [0,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,0,z+1/2 [u,0,w]</td>
</tr>
<tr>
<td></td>
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<td>0,x,z+1/2 [0,u,w]</td>
</tr>
<tr>
<td></td>
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<td>x,x,z+1/2 [u,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>b 3..</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,z+1/2 [0,0,w]</td>
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<td>1/3,2/3,z+1/2 [0,0,w]</td>
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<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>2</td>
<td>a 3.m'</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6m'm'  Along [1,0,0] p1m'1  Along [2,1,0] p1g'1
a* = a   b* = b  a* = (a + 2b)/2  b* = c/2  a* = b/2  b* = c
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
**Origin** on 3m1 at 6,mc

**Asymmetric unit**

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2 \]

**Vertices**

- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 0,0,1
- 1/2,0,1
- 2/3,1/3,1

**Symmetry Operations**

1. \(1\)
   - \((1\,0,0,0)\)

2. \(3^*\)
   - \(0,0,z\)
   - \((3_z\,0,0,0)\)

3. \(3\)
   - \(0,0,z\)
   - \((3_z^{-1}\,0,0,0)\)

4. \(2\)
   - \((0,0,1/2)\)
   - \((2_z\,0,0,1/2)\)

5. \(6\)
   - \((0,0,1/2)\)
   - \((6_z\,0,0,1/2)\)

6. \(6\)
   - \((0,0,1/2)\)
   - \((6_z\,0,0,1/2)\)

7. \(m\)
   - \(x, x, z\)
   - \((m_{xy}\,0,0,0)\)

8. \(m\)
   - \(x, 2x, z\)
   - \((m_x\,0,0,0)\)

9. \(m\)
   - \(2x, x, z\)
   - \((m_{y}\,0,0,0)\)

10. \(c\)
    - \((0,0,1/2)\)
    - \((m_{3}\,0,0,1/2)\)

11. \(c\)
    - \((0,0,1/2)\)
    - \((m_{2}\,0,0,1/2)\)

12. \(c\)
    - \((0,0,1/2)\)
    - \((m_{1}\,0,0,1/2)\)
Generators selected  \((1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).\)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d 1</td>
<td>(1) (x,y,z) [u,v,w] (\vec{u}+v,\vec{u},w)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) (\vec{y},x-y,z) [(v,u-v,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) (x+y,\vec{x},z) [(u+v,\vec{u},w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) (\vec{x},\vec{y},z+1/2) [(u,\vec{v},w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) (y,x+y,z+1/2) [(v,\vec{u}+v,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) (x-y,x,z+1/2) [(u-v,u,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) (\vec{y},\vec{x},z) [(v,u,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) (x+y,y,z) [(u-v,\vec{v},w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(9) (x,x-y,z) [(\vec{u},\vec{u}+v,w)]</td>
</tr>
<tr>
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<td>(10) (y,x,z+1/2) [(\vec{v},\vec{u},w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(11) (x-y,\vec{y},z+1/2) [(\vec{u}+v,\vec{v},w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) (\vec{x},\vec{x}+y,z+1/2) [(u,u-v,\vec{w})]</td>
</tr>
<tr>
<td>6</td>
<td>c .m.</td>
<td>(x,\vec{x},z) [u,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(x,2x,z) [(u,0,0)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\vec{x},\vec{x},z+1/2) [(\vec{u},\vec{u},0)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\vec{x},\vec{x},z+1/2) [u,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>b 3m.</td>
<td>(1/3,2/3,z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2/3,1/3,z+1/2) [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a 3m.</td>
<td>(0,0,z) [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(0,0,z+1/2) [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along \([0,0,1]\)**  \(p6mm\)  
  - \(a^* = a\)  \(b^* = b\)
  - Origin at \(0,0,z\)

- **Along \([1,0,0]\)**  \(p1g11'\)  
  - \(a^* = (a + 2b)/2\)  \(b^* = c\)
  - Origin at \(x,0,0\)

- **Along \([2,1,0]\)**  \(p1m11'\)  
  - \(a^* = b/2\)  \(b^* = c/2\)
  - Origin at \(x,x/2,0\)
Origin on 3m11' at 63 mc1'

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq 1; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \frac{x}{2} \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 & \quad (2) & \quad 3^* 0,0,z & \quad (3) & \quad 3^* 0,0,z \\
(2) & \quad 1 & \quad (3) & \quad 3^* 0,0,z & \quad (3) & \quad 3^* 0,0,z \\
(3) & \quad 0,0,0 & \quad (3) & \quad 0,0,0 & \quad (3) & \quad 0,0,0 \\
(4) & \quad 2 (0,0,1/2) 0,0,z & \quad (5) & \quad 6^* (0,0,1/2) 0,0,z & \quad (6) & \quad 6^* (0,0,1/2) 0,0,z \\
(2) & \quad 0,0,1/2 & \quad (6) & \quad 0,0,1/2 & \quad (6) & \quad 0,0,1/2 \\
(7) & \quad m \times x, x, z & \quad (8) & \quad m \times x, x, z & \quad (9) & \quad m \times 2x, x, z \\
& \quad (m_{xy}|0,0,0) & \quad (m_{xy}|0,0,0) & \quad (m_{xy}|0,0,0) & \quad (m_{xy}|0,0,0) \\
(10) & \quad c (0,0,1/2) x, x, z & \quad (11) & \quad c (0,0,1/2) x, 0, z & \quad (12) & \quad c (0,0,1/2) 0, y, z \\
& \quad (m_3|0,0,1/2) & \quad (m_3|0,0,1/2) & \quad (m_3|0,0,1/2) & \quad (m_3|0,0,1/2)
\end{align*}
\]
For $1'$ + set

\begin{align*}
(1) \, t' & \quad \text{(1) } 0,0,0' \\
(2) \, 3' & \quad 0,0,0 \\
(3) \, 3' & \quad 0,0,0 \\
(4) \, 2' \quad (0,0,1/2) & \quad 0,0,0 \\
(5) \, 6' \quad (0,0,1/2) & \quad 0,0,0 \\
(6) \, 6' \quad (0,0,1/2) & \quad 0,0,0 \\
(7) \, m' \quad x,x,z & \quad (m_x | 0,0,0') \\
(8) \, m' \quad x,2x,z & \quad (m_x | 0,0,0') \\
(9) \, m' \quad 2x,x,z & \quad (m_y | 0,0,0') \\
(10) \, c' \quad (0,0,1/2) \quad x,x,z & \quad (m_x | 0,0,1/2') \\
(11) \, c' \quad (0,0,1/2) \quad x,0,z & \quad (m_y | 0,0,1/2') \\
(12) \, c' \quad (0,0,1/2) \quad 0,y,z & \quad (m_z | 0,0,1/2') \\
\end{align*}

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d</td>
<td>11'</td>
</tr>
<tr>
<td>(1)</td>
<td>x,y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(2)</td>
<td>y,x-y,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(3)</td>
<td>x+y,x,z</td>
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<tr>
<td>(4)</td>
<td>x,y,z+1/2</td>
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<td>(5)</td>
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<td>(6)</td>
<td>x-y,x,z+1/2</td>
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<td>(7)</td>
<td>y,x,z</td>
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<tr>
<td>(8)</td>
<td>x+y,y,z</td>
<td>[0,0,0]</td>
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<tr>
<td>(9)</td>
<td>x-x-y,z</td>
<td>[0,0,0]</td>
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<tr>
<td>(10)</td>
<td>y,x,z+1/2</td>
<td>[0,0,0]</td>
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<tr>
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<td>x-y,y,z+1/2</td>
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<tr>
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<td>x,x+y,z+1/2</td>
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<tr>
<td>6</td>
<td>c</td>
<td>.m.1'</td>
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<td>x,x,z</td>
<td>[0,0,0]</td>
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<tr>
<td></td>
<td>x,2x,z</td>
<td>[0,0,0]</td>
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<tr>
<td></td>
<td>x+2x,z</td>
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</tr>
<tr>
<td></td>
<td>2x,x,z+1/2</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>3m.1'</td>
</tr>
<tr>
<td>(3)</td>
<td>0,0,z</td>
<td>[0,0,0]</td>
</tr>
<tr>
<td>(4)</td>
<td>0,0,z+1/2</td>
<td>[0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = a$</td>
<td>$b^* = b$</td>
</tr>
</tbody>
</table>

Origin at 0,0,z
**Origin** on 3m'1 at 6₃' m'c

**Asymmetric unit**

\[
\begin{align*}
0 & \leq x \leq 2/3; & 0 & \leq y \leq 1/3; & 0 & \leq z \leq 1; & x & \leq (1+y)/2; & y & \leq x/2
\end{align*}
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 & \quad (1^{'}0,0,0) \\
(2) & \quad 3^{*} & \quad 0,0,z & \quad (3_{z}^{*}0,0,0) \\
(3) & \quad 3^{*} & \quad 0,0,z & \quad (3_{z}^{-1}0,0,0) \\
(4) & \quad 2^{'} & \quad (0,0,1/2) & 0,0,z & \quad (2_{z}^{'}0,0,1/2)^{'} \\
(5) & \quad 6^{'} & \quad (0,0,1/2) & 0,0,z & \quad (6_{z}^{'}0,0,1/2)^{'} \\
(6) & \quad 6^{'} & \quad (0,0,1/2) & 0,0,z & \quad (6_{z}^{'}0,0,1/2)^{'} \\
(7) & \quad m^{'} & \quad x,x,z & \quad (m_{x}^{'}0,0,0)^{'} \\
(8) & \quad m^{'} & \quad x,2x,z & \quad (m_{x}^{'}0,0,0)^{'} \\
(9) & \quad m^{'} & \quad 2x,x,z & \quad (m_{y}^{'}0,0,0)^{'} \\
(10) & \quad c & \quad (0,0,1/2) & x,x,z & \quad (m_{x}0,0,1/2) \\
(11) & \quad c & \quad (0,0,1/2) & x,0,z & \quad (m_{y}0,0,1/2) \\
(12) & \quad c & \quad (0,0,1/2) & 0,y,z & \quad (m_{z}0,0,1/2)
\end{align*}
\]
Generators selected  \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7). \)

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 d 1</td>
<td>(1) ( x,y,z ) ([u,v,w])</td>
<td>(2) ( \tilde{y},x-y,z ) ([\tilde{v},u-v,w])</td>
</tr>
<tr>
<td></td>
<td>(4) ( \tilde{x},\tilde{y},z+1/2 ) ([u,v,w])</td>
<td>(5) ( y,x+y,z+1/2 ) ([v,u-v,\tilde{w}])</td>
</tr>
<tr>
<td></td>
<td>(7) ( \tilde{y},\tilde{x},z ) ([\tilde{v},u,w])</td>
<td>(8) ( \tilde{x}+y,y,z ) ([\tilde{u}+v,v,w])</td>
</tr>
<tr>
<td></td>
<td>(10) ( y,x,z+1/2 ) ([v,u,w])</td>
<td>(11) ( x-y,y,z+1/2 ) ([u+v,\tilde{v},\tilde{w}])</td>
</tr>
</tbody>
</table>

| 6 c .m' | \( x,\tilde{x},z \) \([u,\tilde{u},w]\) | \( x,2x,z \) \([u,2u,w]\) | \( 2x,\tilde{x},z \) \([2\tilde{u},\tilde{u},w]\) |

| 2 b 3m' | \( 1/3,2/3,z \) \([0,0,w]\) | \( 2/3,1/3,z+1/2 \) \([0,0,\tilde{w}]\) |

| 2 a 3m' | \( 0,0,z \) \([0,0,w]\) | \( 0,0,z+1/2 \) \([0,0,\tilde{w}]\) |

### Symmetry of Special Projections

- Along \([0,0,1]\)  \( p\bar{6}m\bar{m} \)
  - \( a^* = a \)  \( b^* = b \)
  - Origin at \( 0,0,z \)

- Along \([1,0,0]\)  \( p1g1 \)
  - \( a^* = (a + 2b)/2 \)  \( b^* = c \)
  - Origin at \( x,0,0 \)

- Along \([2,1,0]\)  \( p_{2g}1m1 \)
  - \( a^* = b/2 \)  \( b^* = c/2 \)
  - Origin at \( x,x/2,0 \)
Origin on 3m1 at 63' mc'

Asymmetric unit

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq 1; \quad x \leq (1+y)/2; \quad y \leq x/2\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1 & \quad 1/2,0,1 & \quad 2/3,1/3,1
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1)\ 1 & \quad (2)\ 3^* & \quad (3)\ 3^* \\
(1|0,0,0) & \quad (3;z|0,0,0) & \quad (3;z^{-1}|0,0,0)
\end{align*}
\]

\[
\begin{align*}
(4)\ 2' & \quad (5)\ 6' & \quad (6)\ 6'
\quad (0,0,1/2) \quad 0,0,z & \quad (0,0,1/2) \quad 0,0,z & \quad (0,0,1/2) \quad 0,0,z
\quad (2_z|0,0,1/2)' & \quad (6_z^{-1}|0,0,1/2)' & \quad (6_z|0,0,1/2)'
\end{align*}
\]

\[
\begin{align*}
(7)\ m & \quad (8)\ m & \quad (9)\ m \\
\quad x,x,z & \quad x,2x,z & \quad 2x,x,z
\quad (m_x|0,0,0) & \quad (m_x|0,0,0) & \quad (m_y|0,0,0)
\end{align*}
\]

\[
\begin{align*}
(10)\ c' & \quad (11)\ c' & \quad (12)\ c'
\quad (0,0,1/2) \quad x,x,z & \quad (0,0,1/2) \quad x,0,z & \quad (0,0,1/2) \quad 0,y,z
\quad (m_3|0,0,1/2)' & \quad (m_3|0,0,1/2)' & \quad (m_1|0,0,1/2)'
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>d</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) x-y,z+1/2 [u,v,w]</td>
<td>(5) y,x+1/2 [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x+1/2 [u+v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
<td>(8) x+y,y,z [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,x-y,z [u,u+v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td>(11) x-y,y,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,x+y,z+1/2 [u,u+v,w]</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>c</td>
<td>.m.</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,0]</td>
<td>2x,x,z [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z+1/2 [u,u,0]</td>
<td>2x,x,z+1/2 [0,u,0]</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>3m.</td>
</tr>
<tr>
<td></td>
<td>1/3,2/3,z [0,0,0]</td>
<td>2/3,1/3,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>3m.</td>
</tr>
<tr>
<td></td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p6'mm'  
Along [1,0,0] p1g11'  
Along [2,1,0] p1m1

a* = a  b* = b  
Origin at 0,0,z

a* = (a + 2b)/2  b* = c  
Origin at x,0,0

a* = b/2  b* = c/2  
Origin at x,x/2,0
**Origin** on 3m'1 at 6m'm'

**Asymmetric unit**

\[
\begin{align*}
0 & \leq x \leq 2/3; & 0 & \leq y \leq 1/3; & 0 & \leq z \leq 1; & x & \leq (1+y)/2; & y & \leq x/2
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & 2/3,1/3,1 \\
0,0,1 & & 1/2,0,1
\end{align*}
\]

**Symmetry Operations**

1. \(1 \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (0,0,0)\)
2. \(3^+ \quad 0,0,z \quad (3_z \quad 0,0,0)\)
3. \(3^- \quad 0,0,z \quad (3^{-1} \quad 0,0,0)\)
4. \(2 \quad (0,0,1/2) \quad 0,0,0 \quad (2_z \quad 0,0,1/2)\)
5. \(6 \quad (0,0,1/2) \quad 0,0,0 \quad (6_z^{-1} \quad 0,0,1/2)\)
6. \(6^+ \quad (0,0,1/2) \quad 0,0,0 \quad (6_z \quad 0,0,1/2)\)
7. \(m' \quad x,x,z \quad (m_{xy} \quad 0,0,0)'\)
8. \(m' \quad x,2x,z \quad (m_{x} \quad 0,0,0)'\)
9. \(m' \quad 2x,x,z \quad (m_{y} \quad 0,0,0)'\)
10. \(c' \quad (0,0,1/2) \quad x,x,z \quad (m_{0} \quad 0,0,1/2)'\)
11. \(c' \quad (0,0,1/2) \quad x,0,z \quad (m_{y} \quad 0,0,1/2)'\)
12. \(c' \quad (0,0,1/2) \quad 0,y,z \quad (m_{x} \quad 0,0,1/2)'\)
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
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<th>Site Symmetry</th>
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<tbody>
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<tr>
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<td>(1) x,y,z [u,v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(2) ( \bar{y},x-y,z [\bar{v},u-v,w] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(3) ( x+y,x,z [u+v,\bar{u},w] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(4) ( \bar{x},y,z+1/2 [\bar{u},\bar{v},w] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z+1/2 [v,\bar{u}+v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z+1/2 [u-v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(7) ( \bar{y},x,z [\bar{v},u,w] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(8) ( \bar{x}+y,y,z [u+v,v,w] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(9) x,x-y,z [u,u-v,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(11) x-y,( \bar{y},z+1/2 [u-v,\bar{v},w] )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(12) ( x,x+\bar{y},z+1/2 [\bar{u},u+v,w] )</td>
<td></td>
</tr>
</tbody>
</table>

| 6            | c              | .m'           |
|              | x,\( \bar{x},z [u,\bar{u},w] \)             |
|              | x,\( x,z+1/2 [u,u,w] \)                      |
|              | \( \bar{x},2x,z [u,2u,w] \)                 |
|              | \( \bar{x},z+1/2 [u,2u,w] \)                |
|              | \( 2x,x,z+1/2 [2u,u,w] \)                   |

| 2            | b              | 3m'           |
|              | 1/3,2/3,z [0,0,w] |               |
|              | 2/3,1/3,z+1/2 [0,0,w] |

| 2            | a              | 3m'           |
|              | 0,0,z [0,0,w]  |               |
|              | 0,0,z+1/2 [0,0,w] |

### Symmetry of Special Projections

- **Along [0,0,1]** p6m'm'  
  \( \mathbf{a}^* = \mathbf{a} \) \( \mathbf{b}^* = \mathbf{b} \)  
  Origin at 0,0,z

- **Along [1,0,0]** p1g'1  
  \( \mathbf{a}^* = \mathbf{a} + 2\mathbf{b} \) \( \mathbf{b}^* = \mathbf{c} \)  
  Origin at x,0,0

- **Along [2,1,0]** p1m'1  
  \( \mathbf{a}^* = \mathbf{b} \) \( \mathbf{b}^* = \mathbf{c}/2 \)  
  Origin at x,x/2,0
Origin on $\bar{6}m2$

Asymmetric unit

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq 2y; \quad y \leq \min(1-x, 2x)\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 \\
0,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(4) & \quad m_{x,y,0} \\
(4) & \quad \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(7) & \quad m_{x,x,0} \\
(7) & \quad \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(10) & \quad \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(10) & \quad \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(11) & \quad 2 \begin{pmatrix} x,2x,0 \end{pmatrix} \\
(11) & \quad \begin{pmatrix} 0,0,0 \end{pmatrix} \\
(12) & \quad 2 \begin{pmatrix} 2x,x,0 \end{pmatrix} \\
(12) & \quad \begin{pmatrix} 0,0,0 \end{pmatrix}
\end{align*}
\]
Generators selected

\( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7). \)

Positions

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<tbody>
<tr>
<td>12 o 1</td>
<td>((1) x,y,z [u,v,w])</td>
<td>((2) \bar{y},-x-y,z [v,-u-v,w])</td>
</tr>
<tr>
<td>(4) x,y,z</td>
<td>([u,v,w])</td>
<td>(5) (y,-x-y,z [v,-u+v,w])</td>
</tr>
<tr>
<td>(7) (\bar{y},x,z)</td>
<td>([v,u,w])</td>
<td>(8) (x+y,y,z [u-v,\bar{v},\bar{w}])</td>
</tr>
<tr>
<td>(10) (\bar{y}, \bar{x}, \bar{z})</td>
<td>([v,\bar{u},\bar{w}])</td>
<td>((11) \bar{x}+y,\bar{y},z [u+v,\bar{u},\bar{w}])</td>
</tr>
</tbody>
</table>

6 n ..m. \(x,\bar{z},z [u,u,0]\) | \(x,2x,z [u,0,0]\) | \(2x,\bar{x},z [0,0,0]\) |

6 m m.. \(x,y,1/2 [0,0,w]\) | \(y,-x-y,1/2 [0,0,w]\) | \(x+y,\bar{x},1/2 [0,0,w]\) |

6 l m.. \(\bar{y},y,0 [0,0,w]\) | \(y,-x-y,0 [0,0,w]\) | \(\bar{x}+y,\bar{x},0 [0,0,w]\) |

3 k mm2 \(x,\bar{x},1/2 [0,0,0]\) | \(x,2x,1/2 [0,0,0]\) | \(2x,\bar{x},1/2 [0,0,0]\) |

3 j mm2 \(x,\bar{x},0 [0,0,0]\) | \(x,2x,0 [0,0,0]\) | \(2x,\bar{x},0 [0,0,0]\) |

2 i 3m. \(2/3,1/3,\bar{z} [0,0,0]\) | \(2/3,1/3,\bar{z} [0,0,0]\) | \(2/3,1/3,\bar{z} [0,0,0]\) |

2 h 3m. \(1/3,2/3,\bar{z} [0,0,0]\) | \(1/3,2/3,\bar{z} [0,0,0]\) | \(1/3,2/3,\bar{z} [0,0,0]\) |

2 g 3m. \(0,0,z [0,0,0]\) | \(0,0,z [0,0,0]\) | \(0,0,z [0,0,0]\) |

1 f 6m2 \(2/3,1/3,1/2 [0,0,0]\) | \(2/3,1/3,1/2 [0,0,0]\) | \(2/3,1/3,1/2 [0,0,0]\) |

1 e 6m2 \(2/3,1/3,0 [0,0,0]\) | \(2/3,1/3,0 [0,0,0]\) | \(2/3,1/3,0 [0,0,0]\) |

1 d 6m2 \(1/3,2/3,1/2 [0,0,0]\) | \(1/3,2/3,1/2 [0,0,0]\) | \(1/3,2/3,1/2 [0,0,0]\) |

1 c 6m2 \(1/3,2/3,0 [0,0,0]\) | \(1/3,2/3,0 [0,0,0]\) | \(1/3,2/3,0 [0,0,0]\) |

1 b 6m2 \(0,0,1/2 [0,0,0]\) | \(0,0,1/2 [0,0,0]\) | \(0,0,1/2 [0,0,0]\) |

1 a 6m2 \(0,0,0 [0,0,0]\) | \(0,0,0 [0,0,0]\) | \(0,0,0 [0,0,0]\) |

Symmetry of Special Projections

- Along \([0,0,1]\) 3m11' \(a^* = a \quad b^* = b\) Origin at 0,0,z
- Along \([1,0,0]\) p1m11' \(a^* = c \quad b^* = (a+2b)/2\) Origin at x,0,0
- Along \([2,1,0]\) p2mm \(a^* = c \quad b^* = b/2\) Origin at x,x/2,0
**Origin on \( \overline{6}m21' \)**

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq 2y; \quad y \leq \min(1-x,2x)
\]

**Vertices**

\[
\begin{array}{ccc}
0,0,0 & 2/3,1/3,0 & 1/3,2/3,0 \\
0,0,1/2 & 2/3,1/3,1/2 & 1/3,2/3,1/2
\end{array}
\]

**Symmetry Operations**

For 1 + set

\[
\begin{array}{lll}
(1) & 1 & (2) 3' \quad 0,0,z \\
(1|0,0,0) & (3_z|0,0,0) & (3|0,0,z) \\
(6_z|0,0,0) & (3|0,0,z) & (3_z|0,0,0)
\end{array}
\]

\[
\begin{array}{lll}
(4) & m \quad x,y,0 \\
(m_z|0,0,0) & (5) \overline{6}' \quad 0,0,z; \quad 0,0,0 \\
(6_z|0,0,0) & (6|0,0,z; \quad 0,0,0) & (6_z|0,0,0)
\end{array}
\]

\[
\begin{array}{lll}
(7) & m \quad x,x,z \\
(m_{xy}|0,0,0) & (8) m \quad x,2x,z \\
(m_x|0,0,0) & (9) m \quad 2x,x,z \\
(m_y|0,0,0) & (m_y|0,0,0)
\end{array}
\]

\[
\begin{array}{lll}
(10) & 2 \quad x,x,0 \\
(2|0,0,0) & (11) 2 \quad x,2x,0 \\
(2|0,0,0) & (12) 2 \quad 2x,x,0 \\
(2|0,0,0) & (2|0,0,0)
\end{array}
\]
For 1' + set

<table>
<thead>
<tr>
<th>Multiplicity</th>
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<th>Site Symmetry</th>
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Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

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187.1.1439 - 5 - 3134

Continued 187.2.1440

&  

Symmetry of Special Projections

Along [0,0,1] p3m1'  

a* = a  b* = b
Origin at 0,0,2

Along [1,0,0] p1m1'

a* = c  b* = (a + 2b)/2
Origin at x,0,0

Along [2,1,0] p2mm1'

a* = c  b* = b/2
Origin at x,x/2,0

1  d  6m21'  1/3,2/3,1/2 [0,0,0]
1  c  6m21'  1/3,2/3,0 [0,0,0]
1  b  6m21'  0,0,1/2 [0,0,0]
1  a  6m21'  0,0,0 [0,0,0]
Origin on \( \bar{6}m'2 \)

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x < 2y; \quad y \leq \min(1-x,2x)
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2,0,0 \\
0,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^* \quad 0,0,z \\
(4) & \quad m' \quad x,y,0 \\
(5) & \quad \bar{6}^* \quad 0,0,z; 0,0,0 \\
(6) & \quad \bar{6}^* \quad 0,0,z; 0,0,0 \\
(7) & \quad m' \quad x,x,z \\
(8) & \quad m' \quad x,2x,z \\
(9) & \quad m' \quad 2x,x,z \\
(10) & \quad 2 \quad x,x,0 \\
(11) & \quad 2 \quad x,2x,0 \\
(12) & \quad 2 \quad 2x,x,0
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<thead>
<tr>
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<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
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<td>12 o 1</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) (\bar{y},x,-y,z) [(\bar{v},u-v,w)]</td>
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<tr>
<td></td>
<td></td>
<td>(4) x,y,(\bar{z}) [u,v,w]</td>
<td>(5) (\bar{y},x,-y,\bar{z}) [(\bar{v},u-v,w)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) (\bar{y},\bar{x},z) [(\bar{v},u,w)]</td>
<td>(8) (x+y,y,z) [(\bar{u}+v,v,w)]</td>
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<tr>
<td></td>
<td></td>
<td>(10) (\bar{y},\bar{x},\bar{z}) [(\bar{v},\bar{u},w)]</td>
<td>(11) (x+y,\bar{y},\bar{z}) [(\bar{u}+v,v,w)]</td>
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</tbody>
</table>

\[6 \text{ n} \quad .m'. \]
\[x,\bar{x},z [u,\bar{u},\bar{w}] \quad x,2x,z [u,2u,w] \quad 2x,\bar{x},z [2u,\bar{u},w] \]

\[6 \text{ m} \quad .m'.. \]
\[x,y,1/2 [u,v,0] \quad \bar{y},x-1/2 [\bar{v},u-v,0] \quad x+y,\bar{x},1/2 [\bar{u}+v,\bar{u},0] \]

\[6 \text{ l} \quad .m'.. \]
\[x,y,0 [u,v,0] \quad \bar{y},x,0 [\bar{v},u,0] \quad \bar{y},x,0 [\bar{v},u,0] \quad x+y,\bar{x},0 [\bar{u}+v,\bar{u},0] \]

\[3 \text{ k} \quad m'm'2 \]
\[x,\bar{x},1/2 [u,\bar{u},\bar{0}] \quad x,2x,1/2 [u,2u,0] \quad 2x,\bar{x},1/2 [2u,\bar{u},0] \]

\[3 \text{ j} \quad m'm'2 \]
\[x,\bar{x},0 [u,\bar{u},0] \quad x,2x,0 [u,2u,0] \quad 2x,\bar{x},0 [2u,\bar{u},0] \]

\[2 \text{ i} \quad 3m'. \]
\[2/3,1/3,z [0,0,w] \quad 2/3,1/3,\bar{z} [0,0,\bar{w}] \]

\[2 \text{ h} \quad 3m'. \]
\[1/3,2/3,z [0,0,w] \quad 1/3,2/3,\bar{z} [0,0,\bar{w}] \]

\[2 \text{ g} \quad 3m'. \]
\[0,0,z [0,0,w] \quad 0,0,\bar{z} [0,0,\bar{w}] \]

\[1 \text{ f} \quad \bar{6}'m'2 \]
\[2/3,1/3,1/2 [0,0,0] \quad 2/3,1/3,1/2 [0,0,0] \]

\[1 \text{ e} \quad \bar{6}'m'2 \]
\[2/3,1/3,0 [0,0,0] \quad 2/3,1/3,0 [0,0,0] \]

\[1 \text{ d} \quad \bar{6}'m'2 \]
\[1/3,2/3,1/2 [0,0,0] \quad 1/3,2/3,1/2 [0,0,0] \]

\[1 \text{ c} \quad \bar{6}'m'2 \]
\[1/3,2/3,0 [0,0,0] \quad 1/3,2/3,0 [0,0,0] \]

\[1 \text{ b} \quad \bar{6}'m'2 \]
\[0,0,1/2 [0,0,0] \quad 0,0,1/2 [0,0,0] \]

\[1 \text{ a} \quad \bar{6}'m'2 \]
\[0,0,0 [0,0,0] \quad 0,0,0 [0,0,0] \]

Symmetry of Special Projections

Along [0,0,1] p3m1 
\(a^* = a\) \quad \(b^* = b\)  
Origin at 0,0,z

Along [1,0,0] p1m1 
\(a^* = c\) \quad \(b^* = (a + 2b)/2\)  
Origin at x,0,0

Along [2,1,0] p2m1 
\(a^* = c\) \quad \(b^* = b/2\)  
Origin at x,x/2,0
Origin on $\bar{6}'m2$

Asymmetric unit

\begin{align*}
0 \leq x \leq 2/3; & \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x < 2y; \quad y \leq \min(1-x,2x) \\
\end{align*}

Vertices

\begin{align*}
0,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 \\
0,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/3,2/3,1/2 \\
\end{align*}

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^* \quad 0,0,z \\
(4) & \quad m' \quad x,y,0 \\
(m_x) & \quad 0,0,0 \\
(5) & \quad \bar{6}' \quad 0,0,z; 0,0,0 \\
(6) & \quad \bar{6}' \quad 0,0,z; 0,0,0 \\
(7) & \quad m \quad x,x,z \\
(m_x) & \quad 0,0,0 \\
(8) & \quad m \quad x,2x,z \\
(m_x) & \quad 0,0,0 \\
(9) & \quad m \quad 2x,x,z \\
(m_y) & \quad 0,0,0 \\
(10) & \quad 2' \quad x,x,0 \\
(2) & \quad 0,0,0 \\
(11) & \quad 2' \quad x,2x,0 \\
(2) & \quad 0,0,0 \\
(12) & \quad 2' \quad 2x,x,0 \\
(2) & \quad 0,0,0 \\
\end{align*}
Continued

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
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<tr>
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<th>Coordinates</th>
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<tr>
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<td>(3) x+y,x,z [u+v,u,w]</td>
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<td>(4) x,y,z [u,v,w]</td>
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<td>(8) x+y,y,z [u-v,v,w]</td>
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<td>12 n m'</td>
<td>x,x,z [u,u,0]</td>
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<td>2x,x,z [0,u,0]</td>
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<td>6 m m'</td>
<td>x,y,1/2 [u,v,0]</td>
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<td>y,x-y,1/2 [v,u-v,0]</td>
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<td>x+y,x,1/2 [u+v,u,0]</td>
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Symmetry of Special Projections

Along [0,0,1] p3m1

\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

Along [1,0,0] p1m11'

\[ a^* = c \quad b^* = (a + 2b)/2 \]

Origin at x,0,0

Along [2,1,0] p2'2mm'

\[ a^* = b/2 \quad b^* = c \]

Origin at x,x/2,0
Origin on $\bar{6}m'2'$

**Asymmetric unit**

- $0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq 2y; \quad y \leq \min(1-x,2x)$

**Vertices**

- $0,0,0$  
- $2/3,1/3,0$  
- $1/3,2/3,0$  
- $0,0,1/2$  
- $2/3,1/3,1/2$  
- $1/3,2/3,1/2$  

**Symmetry Operations**

1. $1$
   - $(1|0,0,0)$
2. $3^*$  
   - $0,0,z$  
   - $(3_z|0,0,0)$
3. $3^*$  
   - $0,0,z$  
   - $(3_z^{-1}|0,0,0)$
4. $m$  
   - $x,y,0$  
   - $(m_z|0,0,0)$
5. $\bar{6}^*$  
   - $0,0,z; 0,0,0$  
   - $(6_z^{-1}|0,0,0)$
6. $\bar{6}^*$  
   - $0,0,z; 0,0,0$  
   - $(6_z|0,0,0)$
7. $m'$  
   - $x,x,z$  
   - $(m_{xy}|0,0,0)'$
8. $m'$  
   - $x,2x,z$  
   - $(m_x|0,0,0)'$
9. $m'$  
   - $2x,x,z$  
   - $(m_y|0,0,0)'$
10. $2'$  
    - $x,x,0$  
    - $(2_z|0,0,0)'$
11. $2'$  
    - $x,2x,0$  
    - $(2_z|0,0,0)'$
12. $2'$  
    - $2x,x,0$  
    - $(2_z|0,0,0)'$
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

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</tr>
<tr>
<td>6 n m'</td>
<td>x,x,z [u,u,w]</td>
<td>x,2x,z [u,2u,w]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [u,u,w]</td>
<td>x,2x,z [u,2u,w]</td>
</tr>
<tr>
<td>6 m m..</td>
<td>x,y,1/2 [0,0,w]</td>
<td>y,x-y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>y,x,1/2 [0,0,w]</td>
<td>x+y,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>6 l m..</td>
<td>x,y,0 [0,0,w]</td>
<td>y,x-y,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>y,x,0 [0,0,w]</td>
<td>x+y,y,0 [0,0,w]</td>
</tr>
<tr>
<td>3 k mm'2'</td>
<td>x,x,1/2 [0,0,w]</td>
<td>x,2x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>3 j mm'2'</td>
<td>x,x,0 [0,0,w]</td>
<td>x,2x,0 [0,0,w]</td>
</tr>
<tr>
<td>2 i 3m'</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>2 h 3m'</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>2 g 3m'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>1 f 6m'2'</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>1 e 6m'2'</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>1 d 6m'2'</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>1 c 6m'2'</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td>1 b 6m'2'</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
</tr>
<tr>
<td>1 a 6m'2'</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p3m11'
  - \(a^* = a\) \(b^* = b\)
  - Origin at 0,0,z

- **Along [1,0,0]**: p1m1
  - \(a^* = c\) \(b^* = (a+2b)/2\)
  - Origin at x,0,0

- **Along [2,1,0]**: p2'2mm'
  - \(a^* = c\) \(b^* = b/2\)
  - Origin at x,x/2,0
**Origin** on $\overline{6}m2$

**Asymmetric unit**

- $0 \leq x \leq 2/3$; $0 \leq y \leq 2/3$; $0 \leq z \leq 1/2$; $x < 2y$; $y < \min(1-x,2x)$

**Vertices**

- $0,0,0$
- $2/3,1/3,0$
- $1/3,2/3,0$
- $0,0,1/2$
- $2/3,1/3,1/2$
- $1/3,2/3,1/2$

**Symmetry Operations**

For $(0,0,0) +$ set

1. $1$
2. $3^e$; $0,0,z$
3. $3m$; $0,0,z$
4. $m_x,y,0$
5. $\overline{6}m$; $0,0,z; 0,0,0$
6. $\overline{6}m$; $0,0,z; 0,0,0$
7. $m_{xy}$; $0,0,0$
8. $m_x$; $x,2x,0$
9. $m_y$; $x,2x,0$
10. $m_{xy}$; $0,0,0$

**Diagram**

- P2$_c$6m2
- $\overline{6}m2'$
- Hexagonal

187.6.1444 - 3 - 3141
For \((0,0,1)' + \) set

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1) t'(0,0,1))</td>
<td>((0,0,0) + (0,0,1)' +)</td>
<td>((2) 3'(0,0,1))</td>
<td>((0,0,1)')</td>
</tr>
<tr>
<td>((1</td>
<td>0,0,1))'</td>
<td></td>
<td>((3) 3'(0,0,1))</td>
</tr>
<tr>
<td>((4) m' x,y,1/2)</td>
<td></td>
<td>((5) \delta' 0,0,0; 0,0,1/2)</td>
<td>((0,0,1)')</td>
</tr>
<tr>
<td>((m_m</td>
<td>0,0,1)')</td>
<td></td>
<td>((6) \delta' 0,0,0; 0,0,1/2)</td>
</tr>
<tr>
<td>((7) c' (0,0,1))</td>
<td></td>
<td>((8) c' (0,0,1))</td>
<td>((0,0,1)')</td>
</tr>
<tr>
<td>((m_x</td>
<td>0,0,1)')</td>
<td></td>
<td>((9) c' (0,0,1))</td>
</tr>
<tr>
<td>((10) 2' x,x,1/2)</td>
<td></td>
<td>((11) 2' x,2x,1/2)</td>
<td>((0,0,1)')</td>
</tr>
<tr>
<td>((2_1</td>
<td>0,0,1)')</td>
<td></td>
<td>((12) 2' 2x,x,1/2)</td>
</tr>
</tbody>
</table>

Generators selected

\((1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).\)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>o</td>
<td>1</td>
</tr>
<tr>
<td>12</td>
<td>n</td>
<td>m'.</td>
</tr>
<tr>
<td>12</td>
<td>l</td>
<td>m..</td>
</tr>
<tr>
<td>6</td>
<td>k</td>
<td>m'2'</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>m2</td>
</tr>
<tr>
<td>4</td>
<td>i</td>
<td>3m.</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>3m.</td>
</tr>
<tr>
<td>4</td>
<td>g</td>
<td>3m.</td>
</tr>
<tr>
<td>2</td>
<td>f</td>
<td>(\delta'2)</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>(\delta2)</td>
</tr>
</tbody>
</table>

Continued 187.6.1444

P\(_{2_1}\bar{6}m2\)

187.6.1444 - 4 - 3142
2 d 6'm2' 1/3,2/3,1/2 [0,0,0]
2 c 6m2 1/3,2/3,0 [0,0,0]
2 b 6'm2' 0,0,1/2 [0,0,0]
2 a 6m2 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p3m11'
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b} \)
Origin at 0,0,z

Along [1,0,0] p1m11'
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)
Origin at x,0,0

Along [2,1,0] p2mm
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)
Origin at x,x/2,0
Origin on $\bar{6}m2$

Asymmetric unit

$0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/2; \quad x \leq 2y; \quad y \leq \min(1-x,2x)$

Vertices

$0,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0$

$0,0,1/2 \quad 2/3,1/3,1/2 \quad 1/3,2/3,1/2$

Symmetry Operations

For $(0,0,0) + \text{set}$

(1) 1

(2) $3^+ \quad 0,0,z$

(3) $3^- \quad 0,0,z$

(4) $m' \quad x,y,0$

(5) $\bar{6}^+ \quad 0,0,z; 0,0,0$

(6) $\bar{6}^- \quad 0,0,z; 0,0,0$

(7) $m' \quad x,x,z$

(8) $m' \quad x,2x,z$

(9) $m' \quad 2x,x,z$

(10) $2 \quad x,x,0$

(11) $2 \quad x,2x,0$

(12) $2 \quad 2x,x,0$
For $(0,0,1)' + \text{set}

<table>
<thead>
<tr>
<th>(1) t' (0,0,1)</th>
<th>(2) 3'(0,0,1)</th>
<th>(3) 3'(0,0,1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (0,0,1)</td>
<td>0,0,z</td>
<td>0,0,z</td>
</tr>
<tr>
<td>(3) t (0,0,1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(4) m x,y,1/2</th>
<th>(5) 6' 0,0,z</th>
<th>(6) 6' 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m_x,0,0,1)</td>
<td>0,0,1/2</td>
<td>0,0,1/2</td>
</tr>
<tr>
<td>(6) z(0,0,1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(7) c (0,0,1)</th>
<th>(8) c (0,0,1)</th>
<th>(9) c (0,0,1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m_y,0,0,1)</td>
<td>x,2x,z</td>
<td>2x,x,z</td>
</tr>
<tr>
<td>(m_y,0,0,1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(10) 2' x,x,1/2</th>
<th>(11) 2' x,2x,1/2</th>
<th>(12) 2' x,x,1/2</th>
</tr>
</thead>
<tbody>
<tr>
<td>2x,2x,1/2</td>
<td></td>
<td>2x,2x,1/2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2x,2x,1/2</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,0,1)' +</td>
<td></td>
</tr>
<tr>
<td>24 o 1 x,y,z [u,v,w]</td>
<td>(0,0,0) + (0,0,1)' +</td>
</tr>
<tr>
<td>4 h 3m'. 1/3,2/3,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 i 3m'. 2/3,1/3,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 g 3m'. 0,0,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>6 j m'm'2 2x,0 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>6 k mm'2' x,x,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>12 l m'.. x,y,0 [u,v,0]</td>
<td></td>
</tr>
<tr>
<td>12 m m.. x,y,1/2 [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>12 n .m'. x,x,z [u,u,w]</td>
<td></td>
</tr>
<tr>
<td>12 l m'.. y,x,0 [v,u,0]</td>
<td></td>
</tr>
<tr>
<td>6 f .6m'2' 2x,0 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>2 e .6m'2 2x,0 [u,u,0]</td>
<td></td>
</tr>
</tbody>
</table>

187.7.1445 - 2 - 3145
Continued 187.7.1445

2  d  \(\overline{6}m'2'\)  1/3,2/3,1/2 [0,0,w]
2  c  \(\overline{6}'m'2\)  1/3,2/3,0 [0,0,0]
2  b  \(\overline{6}m'2'\)  0,0,1/2 [0,0,w]
2  a  \(\overline{6}'m'2\)  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p3m11'  
\(a^* = a\)  \(b^* = b\)  
Origin at 0,0,z

Along [1,0,0] \(p_{2a}1m'1\)  
\(a^* = c\)  \(b^* = (a + 2b)/2\)  
Origin at x,0,1/2

Along [2,1,0] \(p_{2a}2m'm'\)  
\(a^* = c\)  \(b^* = b/2\)  
Origin at x,x/2,0
**Origin** on 3c2

**Asymmetric unit**

\[ 0 < x < 2/3; \quad 0 < y < 2/3; \quad 0 < z < 1/4; \quad x < (1+y)/2; \quad y \leq \min(1-x,(1+x)/2) \]

**Vertices**

\[
\begin{array}{cccccc}
0,0,0 & 1/2,0,0 & 2/3,1/3,0 & 1/3,2/3,0 & 0,1/2,0 \\
0,0,1/4 & 1/2,0,1/4 & 2/3,1/3,1/4 & 1/3,2/3,1/4 & 0,1/2,1/4 \\
\end{array}
\]

**Symmetry Operations**

1. \(1\)
   - \((1 | 0,0,0)\)

2. \(3^+\)
   - \((0,0,z)\)
   - \((3_z | 0,0,0)\)

3. \(3^-\)
   - \((0,0,z)\)
   - \((3_z^{-1} | 0,0,0)\)

4. \(m\) \(x,y,1/4\)
   - \((m_z | 0,0,1/2)\)

5. \(\bar{6}^-\)
   - \((0,0,z; 0,0,1/4)\)
   - \((6_z^{-1} | 0,0,1/2)\)

6. \(\bar{6}^+\)
   - \((0,0,z; 0,0,1/4)\)
   - \((6_z | 0,0,1/2)\)

7. \(c\) \((0,0,1/2)\)
   - \((m_y | 0,0,1/2)\)

8. \(c\) \((0,0,1/2)\)
   - \((x,2x,z)\)
   - \((m_z | 0,0,1/2)\)

9. \(c\) \((0,0,1/2)\)
   - \((0,0,1)\)
   - \((x,2x,z)\)
   - \((m_y | 0,0,1/2)\)

10. \(2\) \(x,x,0\)
    - \((2 | 0,0,0)\)

11. \(2\) \(x,2x,0\)
    - \((2 | 0,0,0)\)

12. \(2\) \(2x,x,0\)
    - \((2 | 0,0,0)\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>l</td>
</tr>
<tr>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y, x-y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y, x-z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x,y,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+y,x,z+1/2 [u,v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u+w]</td>
</tr>
<tr>
<td></td>
<td>(8) x+y,y,z+1/2 [u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,x-y,z+1/2 [u,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x+y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x-x-z [u,u-v,w]</td>
</tr>
</tbody>
</table>

6 k       | m.          |
| x,y,1/4  | [0,0,w]    |
|          | y,x-y,1/4 [0,0,w] |
|          | x+y,x,1/4 [0,0,w] |
|          | x,x-y,3/4 [0,0,w] |

6 j       | ..2         |
| x,x,0    | [u,u,0]    |
|          | x,2x,0 [u,2u,0] |
|          | 2x,x,0 [2u,u,0] |
|          | x,2x,1/2 [u,2u,0] |
|          | 2x,x,1/2 [2u,u,0] |

4 i       | 3..         |
| 2/3,1/3,z| [0,0,w]    |
| 2/3,1/3,z+1/2 | [0,0,w] |
| 2/3,1/3,z+1/2 | [0,0,w] |
| 2/3,1/3,z | [0,0,w] |

4 h       | 3..         |
| 1/3,2/3,z| [0,0,w]    |
| 1/3,2/3,z+1/2 | [0,0,w] |
| 1/3,2/3,z+1/2 | [0,0,w] |
| 1/3,2/3,z | [0,0,w] |

4 g       | 3..         |
| 0,0,z    | [0,0,w]    |
| 0,0,z+1/2 | [0,0,w] |
| 0,0,z+1/2 | [0,0,w] |
| 0,0,z    | [0,0,w] |

2 f       | 6..         |
| 2/3,1/3,1/4| [0,0,w] |
| 2/3,1/3,3/4| [0,0,w] |

2 e       | 3.2         |
| 2/3,1/3,0 | [0,0,0]    |
| 2/3,1/3,1/2 | [0,0,0] |

2 d       | 6..         |
| 1/3,2/3,1/4| [0,0,w] |
| 1/3,2/3,3/4| [0,0,w] |

2 c       | 3.2         |
| 1/3,2/3,0 | [0,0,0]    |
| 1/3,2/3,1/2 | [0,0,0] |

2 b       | 6..         |
| 0,0,1/4  | [0,0,w]    |
| 0,0,3/4  | [0,0,w]    |

2 a       | 3.2         |
| 0,0,0    | [0,0,0]    |
| 0,0,1/2  | [0,0,0]    |

Symmetry of Special Projections

Along [0,0,1] p3m11'  
a* = a  b* = b  
Origin at 0,0,z

Along [1,0,0] p3m11  
a* = c/2  b* = (a + 2b)/2  
Origin at 0,0,1/4

Along [2,1,0] p2mg  
a* = c  b* = b/2  
Origin at x,0,1/4

Origin at x,x/2,0
**Origin** on \(3c21'\)

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,(1+x)/2)
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/4 & \quad 1/2,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/3,2/3,1/4 & \quad 0,1/2,1/4
\end{align*}
\]

**Symmetry Operations**

For \(1 \neq \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3 \quad 0,0,z \\
(4) & \quad m \quad x,y,1/4 \\
(5) & \quad 6^* \quad 0,0,z; 0,0,1/4 \\
(6) & \quad 6 \quad 0,0,z; 0,0,1/4 \\
(7) & \quad c \quad (0,0,1/2) \quad x,x,z \\
(8) & \quad c \quad (0,0,1/2) \quad x,2x,z \\
(9) & \quad c \quad (0,0,1/2) \quad 2x,x,z \\
(10) & \quad 2 \quad x,x,0 \\
(11) & \quad 2 \quad x,2x,0 \\
(12) & \quad 2 \quad 2x,x,0
\end{align*}
\]
Continued

For 1’ + set

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<th>(2) 3’</th>
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<table>
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<th>x,y,1/4</th>
<th>(5) 6’</th>
<th>0,0,z, 0,0,1/4</th>
<th>(6) 6’</th>
<th>0,0,z, 0,0,1/4</th>
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<tbody>
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<td>(m,)</td>
<td>0,0,1/2</td>
<td>(6,)</td>
<td>0,0,1/2</td>
<td>(6,)</td>
<td>0,0,1/2</td>
</tr>
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<table>
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<th>(7) c’</th>
<th>(0,0,1/2)</th>
<th>x,x,z</th>
<th>(8) c’</th>
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<th>x,2x,z</th>
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<tr>
<td>(m,)</td>
<td>0,0,1/2</td>
<td>(m,)</td>
<td>0,0,1/2</td>
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Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1’.

Positions

Multiplicity
Wyckoff letter
Site Symmetry

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<tr>
<th>Point</th>
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<td>12</td>
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<tr>
<td>(2) y,x-y,z</td>
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</tr>
<tr>
<td>(3) x+y,x,z</td>
<td>[0,0,0]</td>
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</tr>
<tr>
<td>(4) x,y,z+1/2</td>
<td>[0,0,0]</td>
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<tr>
<td>(5) y,x,y,z+1/2</td>
<td>[0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(6) x+y,x,z+1/2</td>
<td>[0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(7) y,x,z+1/2</td>
<td>[0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(8) x+y,y,z+1/2</td>
<td>[0,0,0]</td>
<td></td>
</tr>
<tr>
<td>(9) x,y,x,z+1/2</td>
<td>[0,0,0]</td>
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</tr>
<tr>
<td>(10) y,x,z</td>
<td>[0,0,0]</td>
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</tr>
<tr>
<td>(11) x+y,y,z</td>
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<td>x,y,1/4</td>
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<td>x+y,x,1/4</td>
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<td>2x,x,1/2</td>
</tr>
<tr>
<td>2/3,1/3,z</td>
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<tr>
<td>(2,2)</td>
<td>0,0,0</td>
<td>2/3,1/3,z+1/2</td>
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<tr>
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<td>(2,2)</td>
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<td>0,0,z</td>
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<tr>
<td>2/3,1/3,1/4</td>
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<tr>
<td>(2,2)</td>
<td>0,0,0</td>
<td>0,0,1/2</td>
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</table>
Symmetry of Special Projections

Along [0,0,1] \( p3m11' \)  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0] \( p1m11' \)  
\( \mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)  
Origin at x,0,0

Along [2,1,0] \( p2mg1' \)  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)  
Origin at x,x/2,0
Origin on 3c'2

Asymmetric unit

\[ 0 < x < \frac{2}{3}; \quad 0 < y < \frac{2}{3}; \quad 0 < z < \frac{1}{4}; \quad x < \frac{(1+y)}{2}; \quad y < \min(1-x,\frac{1+x}{2}) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0 \\
0,0,1/4 & \quad 1/2,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/3,2/3,1/4 & \quad 0,1/2,01/4
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) \quad 1 & \quad (2) \quad 3^* \quad 0,0,z \\
(1,0,0,0) & \quad (3,0,0,0) & \quad (3,0,0,0) \\
(4) \quad m' \quad x,y,1/4 & \quad (5) \quad \bar{6}' \quad 0,0,z; 0,0,1/4 \\
(m_2,0,0,1/2)' & \quad (6,0,0,1/2)' & \quad (6,0,0,1/2)' \\
(7) \quad c' \quad (0,0,1/2) & \quad (8) \quad c' \quad (0,0,1/2) \\
(m_y,0,0,1/2)' & \quad (m_x,0,0,1/2)' & \quad (m_y,0,0,1/2)' \\
(10) \quad 2 \quad x,x,0 & \quad (11) \quad 2 \quad x,2x,0 \\
(2,0,0,0) & \quad (2,0,0,0) & \quad (2,0,0,0)
\end{align*}
\]

188.3.1448 - 1 - 3152
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

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<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
<th>Coordinates</th>
<th>Coordinates</th>
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<td>i</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [u-v,w]</td>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<td></td>
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<td>(4) x,y,z+1/2 [u,v,w]</td>
<td>(5) y,x-y,z+1/2 [u-v,w]</td>
<td>(6) x+y,x,z+1/2 [u+v,u,w]</td>
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<td>(7) y,x,z+1/2 [v,u,0]</td>
<td>(8) x+y,y,z+1/2 [u+v,v,w]</td>
<td>(9) x,x-y,z+1/2 [v,u-v,w]</td>
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<td>k</td>
<td>m'</td>
<td>x,y,1/4 [u,v,0]</td>
<td>y,x-y,1/4 [u-v,0]</td>
<td>x+y,x,1/4 [u+v,u,0]</td>
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<td>y,x,3/4 [v,u,0]</td>
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<td>x,x,1/2 [u,u,0]</td>
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<td>0,0,z+1/2 [0,0,w]</td>
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<td>1/3,2,3,1/2 [0,0,0]</td>
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<td>0,0,1/4 [0,0,0]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p3m1
a* = a b* = b
Origin at 0,0,z

Along [1,0,0] p1m1
a* = c/2 b* = (a + 2b)/2
Origin at x,0,0

Along [2,1,0] p2m1g'
a* = c b* = b/2
Origin at x,x/2,0
**Origin** on 3c2'  

**Asymmetric unit**  
\[0 < x < \frac{2}{3}; \quad 0 < y < \frac{2}{3}; \quad 0 < z < \frac{1}{4}; \quad x < \frac{(1+y)}{2}; \quad y < \min(1-x,(1+x)/2)\]

**Vertices**  
0,0,0 \quad \frac{1}{2},0,0 \quad \frac{2}{3},\frac{1}{3},0 \quad \frac{1}{3},\frac{2}{3},0 \quad 0,\frac{1}{2},0 \quad 0,0,\frac{1}{4} \quad \frac{1}{2},0,\frac{1}{4} \quad \frac{2}{3},\frac{1}{3},\frac{1}{4} \quad \frac{1}{3},\frac{2}{3},\frac{1}{4} \quad 0,\frac{1}{2},0\frac{1}{4}

**Symmetry Operations**

(1) 1  
(1) 0,0,0

(2) \(3^*\) 0,0,\(z\)  
(3) \(3^{-1}\) 0,0,\(z\)

(3) \(3^{-1}\) 0,0,\(z\)

(4) \(m'\) \(x,y,\frac{1}{4}\)  
\((m_{y}z)|0,0,\frac{1}{2}\)'  
\((m_{x}z)|0,0,\frac{1}{2}\)'

(5) \(\overline{6}'\) 0,0,\(z\); 0,0,1/4  
\((6_{z}^{-1})|0,0,\frac{1}{2}\)'  
\((6_{z})|0,0,\frac{1}{2}\)'

(6) \(\overline{6}'\) 0,0,\(z\); 0,0,1/4  
\((6_{z})|0,0,\frac{1}{2}\)'

(7) \(c\) \((0,0,1/2)\) \(x,y,z\)  
\((m_{x}z)|0,0,\frac{1}{2}\)'

(8) \(c\) \((0,0,1/2)\) \(x,2x,z\)  
\((m_{x}|0,0,\frac{1}{2})\)

(9) \((c(0,0,1/2))\) 2x,x,z  
\((m_{y}|0,0,\frac{1}{2})\)

(10) \(2'\) \(x,x,0\)  
\((2_{1}|0,0,0)\)'  

(11) \(2'\) \(x,2x,0\)  
\((2_{1}|0,0,0)\)'

(12) \(2'\) \(2x,x,0\)  
\((2_{1}|0,0,0)\)'

188.4.1449 - 1 - 3154
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Generators</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
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<td>12</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) y,x-y,z [v,u-v,w]</td>
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<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>(4) x,y,z+1/2 [u,v,w]</td>
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<td>(4) x,y,z+1/2 [u,v,w]</td>
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<td>(5) y,x-y,z+1/2 [v,u-v,w]</td>
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<td>(5) y,x-y,z+1/2 [v,u-v,w]</td>
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<tr>
<td>(6) x+y,x,z+1/2 [u+v,u,w]</td>
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<td>(6) x+y,x,z+1/2 [u+v,u,w]</td>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
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<td>(9) x,x-y,z+1/2 [u,u+v,w]</td>
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<td>(10) y,x,z [v,u,w]</td>
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<td>(10) y,x,z [v,u,w]</td>
</tr>
<tr>
<td>(11) x+y,y,z [u,v,v,w]</td>
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<td>(11) x+y,y,z [u,v,v,w]</td>
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<tr>
<td>(12) x,x-y,z [u,u+v,w]</td>
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<td>(12) x,x-y,z [u,u+v,w]</td>
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</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p3m1
a* = a b* = b
Origin at 0,0,z

Along [1,0,0] p3m1
a* = a/2 b* = (a + 2b)/2
Origin at 0,0,0

Along [2,1,0] p2'm'g
a* = c b* = b/2
Origin at 0,0,0
Origin on 3c'2'

Asymmetric unit

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<th>0 ≤ y ≤ 2/3;</th>
<th>0 ≤ z ≤ 1/4;</th>
<th>x ≤ (1+y)/2;</th>
<th>y ≤ min(1-x,(1+x)/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertices</td>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
<td>1/3,2/3,0</td>
<td>0,1/2,0</td>
</tr>
<tr>
<td></td>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
<td>2/3,1/3,1/4</td>
<td>1/3,2/3,1/4</td>
<td>0,1/2,01/4</td>
</tr>
</tbody>
</table>

Symmetry Operations

1. 1
2. 3* 0,0,z
   (3z|0,0,0)
3. 3' 0,0,z
   (3z|0,0,0)
4. m x,y,1/4
   (mz|0,0,1/2)
5. 6* 0,0,z; 0,0,1/4
   (6z|0,0,1/2)
6. 6' 0,0,z; 0,0,1/4
   (6z|0,0,1/2)
7. c' (0,0,1/2) x,x,z
   (mxy|0,0,1/2')
8. c' (0,0,1/2) x,2x,z
   (mx|0,0,1/2')
9. c' (0,0,1/2) 2x,x,z
   (my|0,0,1/2')
10. 2' x,x,0
   (2|0,0,0')
11. 2' x,2x,0
    (2|0,0,0')
12. 2' 2x,x,0
    (2|0,0,0')
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>1</td>
<td>x,y,z [u,v,w]</td>
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<td>l</td>
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<tr>
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<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
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<tr>
<td>1</td>
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<td>(3) x+y,x,z [u+v,u,w]</td>
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</tr>
<tr>
<td>1</td>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td>1</td>
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<td>(5) y,x-y,z+1/2 [v,u+v,w]</td>
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<tr>
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<td>(6) x+y,x,z+1/2 [u-v,u,w]</td>
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<tr>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
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<tr>
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<td>(8) x+y,y,z+1/2 [u+v,v,w]</td>
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<td>(10) y,x,z [v,u,w]</td>
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<tr>
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<td></td>
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<td>x,2x,0 [u,0,w]</td>
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<tr>
<td>4</td>
<td>i</td>
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<td>l</td>
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<td>2/3,1/3,z+1/2 [0,0,w]</td>
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<td>2/3,1/3,z+1/2 [0,0,w]</td>
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<tr>
<td>4</td>
<td>g</td>
<td>0,0,z [0,0,w]</td>
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<tr>
<td>1</td>
<td></td>
<td>0,0,z+1/2 [0,0,w]</td>
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<tr>
<td>1</td>
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<td>0,0,z+1/2 [0,0,w]</td>
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</tr>
<tr>
<td>2</td>
<td>f</td>
<td>2/3,1/3,1/4 [0,0,w]</td>
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<td>l</td>
</tr>
<tr>
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<td>2/3,1/3,1/4 [0,0,w]</td>
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<tr>
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<td>2/3,1/3,1/4 [0,0,w]</td>
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<tr>
<td>2</td>
<td>e</td>
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<td>2/3,1/3,1/2 [0,0,w]</td>
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<tr>
<td>2</td>
<td>d</td>
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<tr>
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<td>1/3,2/3,1/4 [0,0,w]</td>
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<tr>
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<td>l</td>
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<tr>
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<tr>
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<td>1/3,2/3,1/2 [0,0,w]</td>
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</tr>
<tr>
<td>2</td>
<td>b</td>
<td>0,0,1/4 [0,0,w]</td>
<td>2</td>
<td>l</td>
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<tr>
<td>1</td>
<td></td>
<td>0,0,3/4 [0,0,w]</td>
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</tr>
<tr>
<td>1</td>
<td></td>
<td>0,0,3/4 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>0,0,0 [0,0,w]</td>
<td>2</td>
<td>l</td>
</tr>
<tr>
<td>1</td>
<td></td>
<td>0,0,1/2 [0,0,w]</td>
<td></td>
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</tr>
<tr>
<td>1</td>
<td></td>
<td>0,0,1/2 [0,0,w]</td>
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</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p3m11' Along [1,0,0] p1m1 Along [2,1,0] p2'mg'

a* = a b* = b a* = c/2 b* = (a + 2b)/2

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
**Origin** on 62m

**Asymmetric unit**

- \(0 \leq x \leq 2/3;\)  \(0 \leq y \leq 1/2;\)  \(0 \leq z \leq 1/2;\)  \(x \leq (1+y)/2;\)  \(y \leq \min(1-x,x)\)

**Vertices**

- \(0,0,0\)
- \(1/2,0,0\)
- \(2/3,1/3,0\)
- \(1/2,1/2,0\)
- \(0,0,1/2\)
- \(1/2,0,1/2\)
- \(2/3,1/3,1/2\)
- \(1/2,1/2,1/2\)

**Symmetry Operations**

1. 1
2. \(3^+ 0,0,z\)
3. \(3^- 0,0,z\)
   - \((3_z | 0,0,0)\)
   - \((3_z^{-1} | 0,0,0)\)
4. \(m x,y,0\)
   - \((m_2 | 0,0,0)\)
5. \(6^- 0,0,z; 0,0,0\)
   - \((6_z^{-1} | 0,0,0)\)
6. \(6^+ 0,0,z; 0,0,0\)
   - \((6_z | 0,0,0)\)
7. \(2 x,x,0\)
   - \((2_{xy} | 0,0,0)\)
8. \(2 x,0,0\)
   - \((2_x | 0,0,0)\)
9. \(2 0,y,0\)
   - \((2_y | 0,0,0)\)
10. \(m x,x,z\)
    - \((m_3 | 0,0,0)\)
11. \(m x,0,z\)
    - \((m_2 | 0,0,0)\)
12. \(m 0,y,z\)
    - \((m_1 | 0,0,0)\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>l</td>
<td>1</td>
</tr>
<tr>
<td>12</td>
<td>l</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) (\bar{y}, \bar{x}, \bar{y}, \bar{z}, \bar{v}, u-v, w)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y, \bar{x}, \bar{z}, \bar{u}+v, \bar{u}, w</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y, \bar{z}, [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) (\bar{y}, \bar{x}, \bar{z}, [v, \bar{u}+v, \bar{w}])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) (x+y, x, \bar{z}, [u-v, u, w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y, \bar{x}, \bar{z}, [v, u, \bar{w}]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(8) x-y, \bar{y}, \bar{z}, [v-u, \bar{v}, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(9) (x, x+y, \bar{z}, [u, u+v, w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) x, \bar{x}, \bar{z}, [v-u, \bar{w}]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(11) y-x, \bar{z}, [u+v, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) x, x+y, \bar{z}, [u, u-v, w]</td>
</tr>
</tbody>
</table>

| 6            | k              | m..           |
| 6            | j              | m..           |
| 6            | i              | ..m           |
|              |                | 1/3, 2/3, z [0, 0, w] |
|              |                | 1/3, 2/3, \(\bar{z}, [0, 0, w]\) |
|              |                | 2/3, 1/3, z [0, 0, w] |
|              |                | 2/3, 1/3, \(\bar{z}, [0, 0, w]\) |

| 4            | h              | 3..           |
| 3            | g              | m2m           |
| 3            | f              | m2m           |
| 2            | e              | 3.m           |
| 2            | d              | 6..           |
| 2            | c              | 6..           |
| 1            | b              | 62m           |
| 1            | a              | 62m           |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p31m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = a)</td>
<td>(b^* = b)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = c)</td>
<td>(b^* = (a + 2b)/2)</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a^* = c)</td>
<td>(b^* = b/2)</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin on \( \bar{6}2m1' \)**

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x)
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2 & \quad 1/2,1/2,1/2
\end{align*}
\]

**Symmetry Operations**

For \( 1' \) + set

\[
\begin{align*}
(1) & \quad 1 & \quad (2) & \quad 3' & \quad 0,0,z \\
(3) & \quad 3' & \quad 0,0,z \\
(4) & \quad m_{x,y,0} & \quad (5) & \quad 6' & \quad 0,0,z & \quad 0,0,0 \\
& \quad (m_{x,y,0}) & \quad (6) & \quad 6' & \quad 0,0,z & \quad 0,0,0 \\
(7) & \quad 2_{x,x,0} & \quad (8) & \quad 2 & \quad x,0,0 \\
& \quad (2_{x,x,0}) & \quad (9) & \quad 2 & \quad 0,y,0 \\
(10) & \quad m_{x,x,z} & \quad (11) & \quad m & \quad x,0,z \\
& \quad (m_{x,x,z}) & \quad (12) & \quad m & \quad 0,y,z
\end{align*}
\]
For 1' + set

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<th>Coordinates</th>
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<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(1 0,0,0)'</td>
<td>(2) y-x-y,z [0,0,0]</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>(2) y,x-y,z [0,0,0]</td>
</tr>
<tr>
<td>0,0,z</td>
<td>(2) y,x-y,z [0,0,0]</td>
</tr>
<tr>
<td>(3) 3'</td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>0,0,z</td>
<td>(3) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>(4) m'</td>
<td>(4) x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>x,y,0</td>
<td>(5) y,0,z [0,0,0]</td>
</tr>
<tr>
<td>(5) m,0,0)</td>
<td>(6) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>(6) m,0,0'</td>
<td>(6) x+y,x,z [0,0,0]</td>
</tr>
<tr>
<td>(7) 2'</td>
<td>(7) x,0,0 [0,0,0]</td>
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<tr>
<td>x,x-y</td>
<td>(8) y-x,y,z [0,0,0]</td>
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<tr>
<td>(8) m,0,0')</td>
<td>(9) x,x+y,z [0,0,0]</td>
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<tr>
<td>(9) m,0,0'</td>
<td>(9) x,x+y,z [0,0,0]</td>
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<td>(10) m'</td>
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<tr>
<td>(12) m,0,0'</td>
<td>(12) x,x+y,z [0,0,0]</td>
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Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); 1'.

Positions

<table>
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<th>Coordinates</th>
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<td>(2) y,x-y,z [0,0,0]</td>
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<td>(3) x+y,x,z [0,0,0]</td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(5) y,x-y,z [0,0,0]</td>
<td>(6) x+y,x,z [0,0,0]</td>
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<tr>
<td>(7) x,y,z [0,0,0]</td>
<td>(8) x-y,y,z [0,0,0]</td>
</tr>
<tr>
<td>(9) x,x+y,z [0,0,0]</td>
<td>(10) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(11) x-y,x,z [0,0,0]</td>
<td>(12) x,x+y,z [0,0,0]</td>
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<tr>
<td>6 k m..1'</td>
<td>x,y,1/2 [0,0,0]</td>
</tr>
<tr>
<td>y,x,1/2 [0,0,0]</td>
<td>y,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>x-y,x,1/2 [0,0,0]</td>
<td>x-y,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>6 j m..1'</td>
<td>x,y,0 [0,0,0]</td>
</tr>
<tr>
<td>y,x,0 [0,0,0]</td>
<td>y,x,0 [0,0,0]</td>
</tr>
<tr>
<td>x-y,y,0 [0,0,0]</td>
<td>x-y,y,0 [0,0,0]</td>
</tr>
<tr>
<td>x,x+y,0 [0,0,0]</td>
<td>x,x+y,0 [0,0,0]</td>
</tr>
<tr>
<td>6 i ..m1'</td>
<td>x,0,z [0,0,0]</td>
</tr>
<tr>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>0,x,z [0,0,0]</td>
<td>0,x,z [0,0,0]</td>
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<tr>
<td>x,x,z [0,0,0]</td>
<td>x,x,z [0,0,0]</td>
</tr>
<tr>
<td>4 h 3..1'</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>1/3,2/3,2 [0,0,0]</td>
<td>1/3,2/3,2 [0,0,0]</td>
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<tr>
<td>2/3,1/3,2 [0,0,0]</td>
<td>2/3,1/3,2 [0,0,0]</td>
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<td>2/3,1/3,2 [0,0,0]</td>
</tr>
<tr>
<td>3 g m2m1'</td>
<td>x,0,1/2 [0,0,0]</td>
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<tr>
<td>0,x,0 [0,0,0]</td>
<td>0,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>0,x,0 [0,0,0]</td>
<td>0,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 f m2m1'</td>
<td>x,0,0 [0,0,0]</td>
</tr>
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<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
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<tr>
<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
</tr>
<tr>
<td>2 e 3.m1'</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>0,0,0 [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>0,0,0 [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d 6..1'</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2/3,1/3,1/2 [0,0,0]</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 6..1'</td>
<td>1/3,2/3,0 [0,0,0]</td>
</tr>
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<td>2/3,1/3,0 [0,0,0]</td>
<td>2/3,1/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b 62m1'</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>
Continued

1 a 62m1' 0,0,0 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p31m1'</td>
<td>a* = a b* = b</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2mm1'</td>
<td>a* = c b* = (a + 2b)/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along [2,1,0]</td>
<td>p1m11'</td>
<td>a* = c b* = b/2</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin on $\bar{6}'2'm$

**Asymmetric unit**

<table>
<thead>
<tr>
<th>Vertices</th>
<th>$0,0,0$</th>
<th>$1/2,0,0$</th>
<th>$2/3,1/3,0$</th>
<th>$1/2,1/2,0$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$0,0,1/2$</td>
<td>$1/2,0,1/2$</td>
<td>$2/3,1/3,1/2$</td>
<td>$1/2,1/2,1/2$</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. $1$
   - $(1|0,0,0)$

2. $3^*$ $0,0,z$
   - $(3_z|0,0,0)$

3. $3^*$ $0,0,z$
   - $(3_z^{-1}|0,0,0)$

4. $m' x,y,0$
   - $(m_2|0,0,0')$

5. $\bar{6}'' - m' x,y,0$ z; $0,0,0$
   - $(6_z^{-1}|0,0,0')$

6. $\bar{6}'' - m' x,y,0$ z; $0,0,0$
   - $(6_z|0,0,0')$

7. $2' x,x,0$
   - $(2_{xy}|0,0,0')$

8. $2' x,x,0$
   - $(2_x|0,0,0')$

9. $2' y,0,0$
   - $(2_y|0,0,0')$

10. $m' x,x,z$
    - $(m_3|0,0,0)$

11. $m' x,x,z$
    - $(m_2|0,0,0)$

12. $m' y,z$
    - $(m_1|0,0,0)$
Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>l</td>
<td>1 (1) x,y,z [u,v,w] (2) y,-x-y,z [v,-u-v,w] (3) x+y,x,z [u+v,u,w] (4) x,y,-z [u,v,w] (5) y,-x-y,z [v,u+v,w] (6) x+y,x,-z [u,u-v,w] (7) y,x,z [v,-u,w] (8) x,y,z [v,w] (9) x,y,z [v+u,v,w] (10) y,x,z [v,u+w] (11) x-y,y,z [v-u,v+w] (12) x-y,x,z [v+u-v,w]</td>
</tr>
<tr>
<td>6</td>
<td>k</td>
<td>m'.. x,y,1/2 [u,v,0] y,x,1/2 [v,u,0]</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>m'.. x,y,0 [u,v,0] y,x,0 [v,u,0]</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>..m x,0,z [u,2u,0] x,0,z [v,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>3.. 1/3,2/3,0 [0,0,w]</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
<td>m'2m x,0,1/2 [u,2u,0]</td>
</tr>
<tr>
<td>3</td>
<td>f</td>
<td>m'2m x,0,0 [u,2u,0]</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>3.m 0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>6'.. 1/3,2/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>6'.. 1/3,2/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>6'2m 0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>6'2m 0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p31m
  - \( \mathbf{a}^* = \mathbf{a} \), \( \mathbf{b}^* = \mathbf{b} \) Origin at 0,0,z

- **Along [1,0,0]**: p2mm
  - \( \mathbf{a}^* = (\mathbf{a} + 2\mathbf{b})/2 \), \( \mathbf{b}^* = \mathbf{c} \) Origin at x,0,0

- **Along [2,1,0]**: p1m11'
  - \( \mathbf{a}^* = \mathbf{c} \), \( \mathbf{b}^* = \mathbf{b}/2 \) Origin at x,x/2,0
Origin on $\bar{6}2m'$

Asymmetric unit
- $0 \leq x \leq 2/3$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$; $x \leq (1+y)/2$; $y \leq \min(1-x,x)$
- Vertices: $0,0,0$, $1/2,0,0$, $2/3,1/3,0$, $1/2,1/2,0$, $0,0,1/2$, $1/2,0,1/2$, $2/3,1/3,1/2$, $1/2,1/2,1/2$

Symmetry Operations

(1) 1
(2) $3^*$ 0,0,z
(3) $3^*$ 0,0,z
(4) $m'$ 0,0,0
(5) $6$' 0,0,0
(6) $6$' 0,0,0
(7) 2 0,0,0
(8) 2 0,0,0
(9) 2 0,0,0
(10) $m'$ 0,0,0
(11) $m'$ 0,0,0
(12) $m'$ 0,0,0
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>l</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>k</td>
<td>m'..</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>m'..</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>..m'</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>3..</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
<td>m'2m'</td>
</tr>
<tr>
<td>3</td>
<td>f</td>
<td>m'2m'</td>
</tr>
<tr>
<td>2</td>
<td>e</td>
<td>3.m'</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>6'..</td>
</tr>
<tr>
<td>2</td>
<td>c</td>
<td>6'..</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>6'2m'</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>6'2m'</td>
</tr>
</tbody>
</table>

### Coordinates

<table>
<thead>
<tr>
<th>12</th>
<th>l</th>
<th>1</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) y,x-y,z [v-u,v,w]</th>
<th>(3) x+y,x,z [u+v,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>k</td>
<td>m'..</td>
<td>x,y,1/2 [u,v,0]</td>
<td>y,x,1/2 [v-u,v,0]</td>
<td>x+y,x,1/2 [u+v,u,0]</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>m'..</td>
<td>x,y,0 [u,v,0]</td>
<td>y,x-y,0 [v-u,v,0]</td>
<td>x+y,x,0 [u+v,u,0]</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>..m'</td>
<td>x,0,z [u,0,w]</td>
<td>0,x,z [0,u,w]</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>4</td>
<td>h</td>
<td>3..</td>
<td>1/3,2,3/z [0,0,w]</td>
<td>1/3,2,3/z [0,0,w]</td>
<td>2/3,1,3/z [0,0,w]</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
<td>m'2m'</td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
<td>x,x,1/2 [u,u,0]</td>
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<tr>
<td>3</td>
<td>f</td>
<td>m'2m'</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
<td>x,x,o [u,u,o]</td>
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<tr>
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<td>e</td>
<td>3.m'</td>
<td>0,0,2 [0,0,w]</td>
<td>0,0,2 [0,0,w]</td>
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</tr>
<tr>
<td>2</td>
<td>d</td>
<td>6'..</td>
<td>1/3,2,3/1 [0,0,0]</td>
<td>2/3,1,3/1 [0,0,0]</td>
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</tr>
<tr>
<td>2</td>
<td>c</td>
<td>6'..</td>
<td>1/3,2,3/0 [0,0,0]</td>
<td>2/3,1,3/0 [0,0,0]</td>
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</tr>
<tr>
<td>1</td>
<td>b</td>
<td>6'2m'</td>
<td>0,0,1/2 [0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>6'2m'</td>
<td>0,0,0 [0,0,0]</td>
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</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p31m'</th>
<th>Along [1,0,0]</th>
<th>p2m'2m'</th>
<th>Along [2,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
<td>a* = c</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
Origin on $\overline{6}2'm'$

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq 2/3; & 0 \leq y & \leq 1/2; & 0 \leq z & \leq 1/2; & x & \leq (1+y)/2; & y & \leq \min(1-x,x) \\
\text{Vertices} & & & & & & & \\
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/2,1/2,0 \\
0,0,1/2 & & 1/2,0,1/2 & & 2/3,1/3,1/2 & & 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1') & \quad 0,0,0 \\
(2) & \quad 3^* \quad 0,0,z \\
(2') & \quad 3 \quad 0,0,0 \\
(3) & \quad 3^* \quad 0,0,z \\
(3') & \quad 3 \quad 0,0,0 \\
(4) & \quad m \quad x,y,0 \\
& \quad (m_2|0,0,0) \\
(5) & \quad 6' \quad 0,0,z; 0,0,0 \\
& \quad (6_2|0,0,0) \\
(6) & \quad 6^* \quad 0,0,z; 0,0,0 \\
& \quad (6_z|0,0,0) \\
(7) & \quad 2' \quad x,x,0 \\
& \quad (2_y|0,0,0)' \\
(8) & \quad 2' \quad x,0,0 \\
& \quad (2_x|0,0,0)' \\
(9) & \quad 2' \quad 0,y,0 \\
& \quad (2_y|0,0,0)' \\
(10) & \quad m' \quad x,x,z \\
& \quad (m_3|0,0,0)' \\
(11) & \quad m' \quad x,0,z \\
& \quad (m_2|0,0,0)' \\
(12) & \quad m' \quad 0,y,z \\
& \quad (m_1|0,0,0)'
\end{align*}
\]
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>1</td>
<td>1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) (\bar{y},x-y,z [\bar{v},u-v,w])</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(3) (x+y,x,z [u+v,\bar{u},w])</td>
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<td>(4) x,y,z [u,v,w]</td>
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<td>(5) (\bar{y},x-y,z [v,u+v,w])</td>
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<tr>
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<td></td>
<td>(6) (x+y,x,z [u-v,u,w])</td>
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<td></td>
<td></td>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(8) (x-y,\bar{y},z [\bar{u}+v,v,w])</td>
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<tr>
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<td></td>
<td>(9) (\bar{x},x+y,z [u,u-v,w])</td>
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<tr>
<td></td>
<td></td>
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<td>(10) y,x,z [v,u,w]</td>
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<td></td>
<td></td>
<td>(11) (x-y,\bar{y},z [u-v,\bar{v},w])</td>
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<td></td>
<td>(12) (\bar{x},x+y,z [u,\bar{u}+v,w])</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>k</td>
<td>m..</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\bar{y},x-y,1/2 [0,0,w])</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(x+y,\bar{x},1/2 [0,0,w])</td>
</tr>
<tr>
<td>6</td>
<td>j</td>
<td>m..</td>
<td>y,x,0 [0,0,w]</td>
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<tr>
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<td></td>
<td></td>
<td>(\bar{y},x-y,0 [0,0,w])</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(x+y,\bar{x},0 [0,0,w])</td>
</tr>
<tr>
<td>6</td>
<td>i</td>
<td>..m'</td>
<td>x,0,z [u,0,w]</td>
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<td></td>
<td></td>
<td>(0,\bar{x},z [0,u,\bar{w}])</td>
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<td></td>
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<td>(\bar{x},\bar{x},z [u,u,w])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>h</td>
<td>3..</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td>3</td>
<td>g</td>
<td>m2'm'</td>
<td>x,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\bar{x},\bar{x},1/2 [0,0,w])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>f</td>
<td>m2'm'</td>
<td>x,0,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(x,x,0 [0,0,w])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>e</td>
<td>3.m'</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,0, (\bar{z} [0,0,w])</td>
</tr>
<tr>
<td>2</td>
<td>d</td>
<td>(\bar{6})..</td>
<td>1/3,2/3,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2/3,1/3,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>c</td>
<td>(\bar{6})..</td>
<td>1/3,2/3,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2/3,1/3,0 [0,0,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>b</td>
<td>(\bar{6}2'm')</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\bar{x},0,1/2 [0,0,w])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a</td>
<td>(\bar{6}2'm')</td>
<td>0,0,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\bar{x},0,0 [0,0,w])</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p31m1'</td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p2'2mm'</td>
</tr>
<tr>
<td>[2,1,0]</td>
<td>p1m1</td>
</tr>
<tr>
<td>a^+ = a</td>
<td>a^+ = c</td>
</tr>
<tr>
<td>b^+ = b</td>
<td>b^+ = (a + 2b)/2</td>
</tr>
<tr>
<td>Origin at 0,0,0</td>
<td>Origin at x,0,0</td>
</tr>
</tbody>
</table>
Origin on $\bar{6}2m$

Asymmetric unit

$0 \leq x \leq 2/3$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$; $x \leq (1+y)/2$; $y \leq \min(1-x, x)$

Vertices

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
<td>1/2,1/2,0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0,0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1/3,1/2</td>
<td>1/2,1/2,1/2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

For $(0,0,0) + \text{set}$

1. $1$
2. $3^*$, $0,0,z$
3. $3$, $0,0,z$
4. $m$, $x,y,0$
5. $\bar{6}^*$, $0,0,z$; $0,0,0$
6. $\bar{6}^*$, $0,0,z$; $0,0,0$
7. $2$, $x,x,0$
8. $2$, $x,0,0$
9. $2$, $0,y,0$
10. $m$, $x,x,z$
11. $m$, $x,0,z$
12. $m$, $0,y,z$

189.6.1456 - 1 - 3169
Continued

For (0,0,1)'+ set

(1) t'(0,0,1)
    (1) 0,0,1)
(2) 3'(0,0,1) 0,0,z
    (3) 3'(0,0,1) 0,0,z
    (3,1) 0,0,1)
(4) m' x,y,1/2
    (m,0,1)'
(5) 6' 0,0,z; 0,0,1/2
    (6) 6' 0,0,z; 0,0,1/2
    (6,1) 0,0,1)'
(7) 2' x,x,1/2
    (2,x,0,1)'
(8) 2' x,0,1/2
    (2,x,0,1)'
(9) 2' 0,y,1/2
    (2,y,0,1)'
(10) c'(0,0,1) x,x,z
    (m,0,1)'
(11) c' (0,0,1) x,0,z
    (m,0,1)'
(12) c' (0,0,1) 0,y,z
    (m,0,1)'

Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>l</td>
<td>1</td>
</tr>
<tr>
<td>12</td>
<td>k</td>
<td>m'.</td>
</tr>
<tr>
<td>12</td>
<td>j</td>
<td>m.</td>
</tr>
<tr>
<td>12</td>
<td>i</td>
<td>..m</td>
</tr>
<tr>
<td>8</td>
<td>h</td>
<td>3.</td>
</tr>
<tr>
<td>6</td>
<td>g</td>
<td>m'2m</td>
</tr>
<tr>
<td>6</td>
<td>f</td>
<td>m2m</td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>3.m</td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>6'..</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>6'..</td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>6'2m</td>
</tr>
</tbody>
</table>

Coordinates

(0,0,0) + (0,0,1)'+

24 l 1
(1) x,y,z [u,v,w]
(2) y, y-x-y,z [u+v,u,w]
(3) x+y, x,z [u+v,u,w]
(4) x,y,z [u,v,w]
(5) y, x-y,z [u+v,u,w]
(6) x+y, x,z [u+v,u,w]
(7) y,x,z [u,v,w]
(8) x-y, y-z [u-v,v,w]
(9) x, x+y, z [u+v,u+w]
(10) y,x,z [u,v,w]
(11) x-y,y,z [u+v,v,w]
(12) x, x+y,z [u+v,u+w]

12 k m'.
(1) x,y,1/2 [u,v,0]
(2) y, x-y,1/2 [v-u,v,0]
(3) x+y, x,1/2 [v-u,v,0]
(4) x,y,z [u,v,w]
(5) y, x-y,z [u+v,u,w]
(6) x+y, x,z [u+v,u,w]
(7) y,x,z [v,u,w]
(8) x-y, y-z [u-v,v,w]
(9) x, x+y, z [u+v,u+w]
(10) y,x,z [v,u,w]
(11) x-y,y,z [u+v,v,w]
(12) x, x+y,z [u+v,u+w]

12 j m.
(1) x,y,0 [0,0,w]
(2) y, x-y,0 [0,0,w]
(3) x+y, x,0 [0,0,w]
(4) y,x,0 [0,0,w]
(5) x-y, y,0 [0,0,w]
(6) x, x+y, 0 [0,0,w]
(7) y,x,0 [0,0,w]
(8) x-y, y,0 [0,0,w]
(9) x, x+y, 0 [0,0,w]
(10) x,y,0 [0,0,w]
(11) y,x,0 [0,0,w]
(12) x, x+y, 0 [0,0,w]

12 i ..m
(1) x,0,z [u,2u,0]
(2) 0,x,z [2u,0,0]
(3) x,0,z [u,0,0]
(4) x,0,0 [0,0,0]
(5) 0,x,0 [0,0,0]
(6) 0,0,z [0,0,0]
(7) 0,0,0 [0,0,0]
(8) 2/3,1/3,0 [0,0,0]
(9) 2/3,1/3,0 [0,0,0]
(10) 2/3,1/3,0 [0,0,0]
(11) 2/3,1/3,0 [0,0,0]
(12) 2/3,1/3,0 [0,0,0]

8 h 3..
(1) 1/3,2/3,z [0,0,0]
(2) 1/3,2/3,z [0,0,0]
(3) 1/3,2/3,z [0,0,0]
(4) 1/3,2/3,z [0,0,0]
(5) 1/3,2/3,z [0,0,0]
(6) 1/3,2/3,z [0,0,0]
(7) 1/3,2/3,z [0,0,0]
(8) 1/3,2/3,z [0,0,0]
(9) 1/3,2/3,z [0,0,0]
(10) 1/3,2/3,z [0,0,0]
(11) 1/3,2/3,z [0,0,0]
(12) 1/3,2/3,z [0,0,0]

6 g m'2m
(1) x,0,1/2 [u,2u,0]
(2) 0,x,1/2 [2u,0,0]
(3) x,0,1/2 [u,2u,0]
(4) 0,x,0 [0,0,0]
(5) 0,x,0 [0,0,0]
(6) 0,x,0 [0,0,0]
(7) 0,x,0 [0,0,0]
(8) 0,x,0 [0,0,0]
(9) 0,x,0 [0,0,0]
(10) 0,x,0 [0,0,0]
(11) 0,x,0 [0,0,0]
(12) 0,x,0 [0,0,0]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Equation 1</th>
<th>Equation 2</th>
<th>Equation 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p31m1'</td>
<td>$a^* = a$</td>
<td>$b^* = b$</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2a* 2mm</td>
<td>$a^* = c$</td>
<td>$b^* = (a + 2b)/2$</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>Along [2,0,0]</td>
<td>p1m11'</td>
<td>$a^* = c$</td>
<td>$b^* = b/2$</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin on \( \bar{6}2m' \)

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x)
\]

**Vertices**

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>2/3,1/3,0</th>
<th>1/2,1/2,0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0,0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1/3,1/2</td>
<td>1/2,1/2,1/2</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

For \((0,0,0) + \) set

- \((1) 1\)
  \((1|0,0,0)\)
- \((2) 3^* \quad 0,0,z\)
  \((3z|0,0,0)\)
- \((3) 3^* \quad 0,0,z\)
  \((3z^{-1}|0,0,0)\)
- \((4) m' \quad x,y,0\)
  \((m_2|0,0,0)')\)
- \((5) \bar{6}^* \quad 0,0,z; 0,0,0\)
  \((\bar{6}_z|0,0,0)')\)
- \((6) \bar{6}^* \quad 0,0,z; 0,0,0\)
  \((\bar{6}_z|0,0,0)')\)
- \((7) 2 \quad x,x,0\)
  \((2_x|0,0,0)\)
- \((8) 2 \quad x,0,0\)
  \((2_y|0,0,0)\)
- \((9) 2 \quad 0,y,0\)
  \((2_y|0,0,0)\)
- \((10) m' \quad x,x,z\)
  \((m_3|0,0,0)')\)
- \((11) m' \quad x,0,z\)
  \((m_2|0,0,0)')\)
- \((12) m' \quad 0,y,z\)
  \((m_1|0,0,0)')\)
Continued

For $(0,0,1)'+ \text{ set}$

<table>
<thead>
<tr>
<th>Generator selected</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) $t'(0,0,1)$</td>
<td>(1) $t'(0,0,1)'$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
<tr>
<td>(1) $t(0,0,1)$</td>
<td>(2) $3^* (0,0,1)$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
<tr>
<td>(1) $t'(0,0,1)'$</td>
<td>(3) $3^* (0,0,1)'$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Generator selected</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4) $m x,y,1/2$</td>
<td>(4) $m x,y,1/2$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
<tr>
<td>(m) $x,y,1/2$</td>
<td>(5) $m x,y,1/2$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
<tr>
<td>(7) $2' x,x,1/2$</td>
<td>(8) $2' x,x,1/2$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
<tr>
<td>(2y) $x,x,1/2'$</td>
<td>(9) $2' x,x,1/2'$</td>
<td>$(0,0,0) + (0,0,1)' +$</td>
</tr>
</tbody>
</table>

Generators selected

(1); $t(1,0,0)$; $t(0,1,0)$; $t'(0,0,1)$; (2); (4); (7).
Continued

2 a  \bar{6}'2m'  0,0,0 [0,0,0]

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p31m1'</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
<td></td>
</tr>
<tr>
<td>[1,0,0]</td>
<td>p_{2a^*}2m'm'</td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>a^* = c</td>
<td>b^* = (a + 2b)/2</td>
<td></td>
</tr>
<tr>
<td>[2,1,0]</td>
<td>p_{2a^*}1m1</td>
<td>Origin at x,x/2,1/2</td>
</tr>
<tr>
<td>a^* = c</td>
<td>b^* = b/2</td>
<td></td>
</tr>
</tbody>
</table>

\[ a^* = \frac{a + 2b}{2} \]
Origin on 32c

Asymmetric unit

\[
\begin{align*}
0 \leq x & \leq 2/3; & 0 \leq y & \leq 2/3; & 0 \leq z & \leq 1/4; & x & \leq (1+y)/2; & y & \leq \min(1-x,(1+x)/2)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 & \quad 0,1/2,0
\end{align*}
\]

\[
\begin{align*}
0,0,1/4 & \quad 1/2,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/3,2/3,1/4 & \quad 0,1/2,1/4
\end{align*}
\]

Symmetry Operations

(1) 1
(1 0,0,0)

(2) 3^* 0,0,z
(3z 0,0,0)

(3) 3^- 0,0,z
(3z^- 0,0,0)

(4) m x,y,1/4
(m_2 0,0,1/2)

(5) 6^- 0,0,z; 0,0,1/4
(6^- 0,0,1/2)

(6) 6^- 0,0,z; 0,0,1/4
(6^- 0,0,1/2)

(7) 2 x,x,0
(2xy 0,0,0)

(8) 2 x,0,0
(2z 0,0,0)

(9) 2 0,y,0
(2y 0,0,0)

(10) c (0,0,1/2) x,x,z
(m_3 0,0,1/2)

(11) c (0,0,1/2) x,0,z
(m_2 0,0,1/2)

(12) c (0,0,1/2) 0,y,z
(m_1 0,0,1/2)
**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Symmetry of Special Projections</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>1/3,2/3,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-z [v,u,w]</td>
<td>1/3,2/3,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
<td>0,0,1/4 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
<td>0,0,1/2 [0,0,0]</td>
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<td></td>
<td>(8) x,y,z [u,v,w]</td>
<td>0,0,3/4 [0,0,0]</td>
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<td>(9) x,y,z [u,v,w]</td>
<td>0,0,1/2 [0,0,0]</td>
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<td>(10) x,y,z [u,v,w]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(11) x,y,z [u,v,w]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(12) x,y,z [u,v,w]</td>
<td>0,0,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>
Origin on 32c1'

Asymmetric unit

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{4}; \quad x \leq \frac{1+y}{2}; \quad y \leq \min(1-x,(1+x)/2)\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 1/3,2/3,0 \quad 0,1/2,0\]
\[0,0,1/4 \quad 1/2,0,1/4 \quad 2/3,1/3,1/4 \quad 1/3,2/3,1/4 \quad 0,1/2,1/4\]

Symmetry Operations

For 1 + set

(1) 1

(2) \(3^*\) 0,0,z
(3) \(3\) 0,0,z

(4) m x,y,1/4

(5) \(\bar{6}^*\) 0,0,z; 0,0,1/4
(6) \(\bar{6}\) 0,0,z; 0,0,1/4

(7) 2 x,x,0
(8) 2 x,0,0
(9) 2 0,y,0

(10) c (0,0,1/2) x,x,z
(11) c (0,0,1/2) x,0,z
(12) c (0,0,1/2) 0,y,z
For 1' + set

<table>
<thead>
<tr>
<th>Position</th>
<th>Generators selected</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1'</td>
<td>(1) t(1,0,0); t(0,1,0); t(0,0,1); (2) (4); (7); 1'.</td>
<td>1 + 1' +</td>
</tr>
<tr>
<td>(2) 3'</td>
<td>(2) y.x-y,z [0,0,0]</td>
<td>(3) x+y,\bar{x},z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(3) y.x-y,z+1/2 [0,0,0]</td>
<td>(4) x+y,\bar{x},z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(4) m'</td>
<td>(5) y.x-y,z+1/2 [0,0,0]</td>
<td>(6) x+y,\bar{x},z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(5) 6'</td>
<td>(5) y.x-y,z [0,0,0]</td>
<td>(7) x+y,\bar{x},z [0,0,0]</td>
</tr>
<tr>
<td>(7) 2'</td>
<td>(6) x+y,\bar{x},z [0,0,0]</td>
<td>(8) x-y,\bar{y},z [0,0,0]</td>
</tr>
<tr>
<td>(8) 2'</td>
<td>(7) x-y,\bar{y},z+1/2 [0,0,0]</td>
<td>(9) x+y,\bar{x},z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(9) 2'</td>
<td>(10) y.x,z+1/2 [0,0,0]</td>
<td>(11) x-y,\bar{y},z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(10) c'</td>
<td>(11) x-y,\bar{y},z [0,0,0]</td>
<td>(12) x+y,\bar{x},z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(11) c'</td>
<td>(12) x+y,\bar{x},z+1/2 [0,0,0]</td>
<td>6 h m..1'</td>
</tr>
<tr>
<td>(12) c'</td>
<td>x,2x,0 [0,0,0]</td>
<td>y,\bar{y},3/4 [0,0,0]</td>
</tr>
<tr>
<td>(13) c'</td>
<td>x,x,1/2 [0,0,0]</td>
<td>x+y,\bar{x},1/2 [0,0,0]</td>
</tr>
<tr>
<td>(14) c'</td>
<td>x,x,1/2 [0,0,0]</td>
<td>x,x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>(15) c'</td>
<td>1/3,2/3,z [0,0,0]</td>
<td>1/3,2/3,z+1/2 [0,0,0]</td>
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<tr>
<td>(16) c'</td>
<td>2/3,1/3,z [0,0,0]</td>
<td>2/3,1/3,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(17) c'</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>(18) c'</td>
<td>0,0,1/2 [0,0,0]</td>
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</tr>
</tbody>
</table>
Continued

Symmetry of Special Projections

Along [0,0,1]  p31m1'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0]  p2mg1'  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)  
Origin at x,0,0

Along [2,1,0]  p1m11'  
\( \mathbf{a}^* = \mathbf{c}/2 \quad \mathbf{b}^* = \mathbf{b}/2 \)  
Origin at x,x/2,0
Origin on 32'c

Asymmetric unit

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0, 1/4</td>
<td>1/2</td>
<td>0</td>
</tr>
<tr>
<td>1/2</td>
<td>0</td>
<td>1/4</td>
</tr>
</tbody>
</table>

Vertices

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 0, 0</td>
<td>1/2, 0, 0</td>
<td>2/3, 1/3, 0</td>
</tr>
<tr>
<td>0, 0, 1/4</td>
<td>1/2, 0, 1/4</td>
<td>2/3, 1/3, 1/4</td>
</tr>
<tr>
<td>0, 1/2, 0</td>
<td>1/3, 2/3, 0</td>
<td>0, 1/2, 0</td>
</tr>
<tr>
<td>0, 1/2, 1/4</td>
<td>1/3, 2/3, 1/4</td>
<td>0, 1/2, 1/4</td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) 1
(1 1 0, 0, 0)

(2) 3+ 0, 0, z
(2 3 0, 0, 0)

(3) 3- 0, 0, z
(3 3- 0, 0, 0)

(4) m' x, y, 1/4
(m 4 0, 0, 1/2)

(5) 6- x, 0, z; 0, 0, 1/4
(5 6 0, 0, 1/2)

(6) 6+ 0, 0, z; 0, 0, 1/4
(6 6 0, 0, 1/2)

(7) 2' x, x, 0
(7 2' 0, 0, 0)

(8) 2' x, 0, 0
(8 2' 0, 0, 0)

(9) 2' y, 0, 0
(9 2' 0, 0, 0)

(10) c (0, 0, 1/2) x, x, z
(c 10 0, 0, 1/2)

(11) c (0, 0, 1/2) x, 0, z
(c 11 0, 0, 1/2)

(12) c (0, 0, 1/2) y, y, z
(c 12 0, 0, 1/2)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>i 1</td>
<td>12</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>h m'..</td>
<td>6</td>
<td>x,y,1/4 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>y,x,3/4 [v,u,0]</td>
</tr>
<tr>
<td>g .2'</td>
<td>6</td>
<td>x,x,0 [u,2u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,1/2 [u,2u,w]</td>
</tr>
<tr>
<td>f 3..</td>
<td>4</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>e 3..</td>
<td>4</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>d 6'..</td>
<td>2</td>
<td>2/3,1/3,1/4 [0,0,0]</td>
</tr>
<tr>
<td>c 6'..</td>
<td>2</td>
<td>1/3,2/3,1/4 [0,0,0]</td>
</tr>
<tr>
<td>b 6'..</td>
<td>2</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td>a 32'</td>
<td>2</td>
<td>0,0,0 [0,0,w]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p31m

a* = a  b* = b

Origin at 0,0,z

Along [1,0,0] p2'm'g

a* = c  b* = (a + 2b)/2

Origin at x,0,0

Along [2,1,0] p2a,1m1

a* = c/2  b* = b/2

Origin at x,x/2,0
**Origin** on 32c'

**Asymmetric unit**

\[
\begin{align*}
0 \leq x & \leq 2/3; & 0 \leq y & \leq 2/3; & 0 \leq z & \leq 1/4; & x & \leq (1+y)/2; & y & \leq \min(1-x,(1+x)/2) \\
\end{align*}
\]

**Vertices**

\[
\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/3,2/3,0 & & 0,1/2,0 \\
0,0,1/4 & & 1/2,0,1/4 & & 2/3,1/3,1/4 & & 1/3,2/3,1/4 & & 0,1/2,1/4 \\
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \ 1 \ & (2) & \ 3^+ & 0,0,z & & (3) & \ 3^- & 0,0,z \\
(1 | 0,0,0) & & (3_z | 0,0,0) & & (3_z | 0,0,0) \\
(4) & \ m' & x,y,1/4 & & (5) & \ 6^- & 0,0,z; 0,0,1/4 & & (6) & \ 6^+ & 0,0,z; 0,0,1/4 \\
(m_2 | 0,0,1/2)' & & (6_z | 0,0,1/2)' & & (6_z | 0,0,1/2)' \\
(7) & \ 2 & x,x,0 & & (8) & \ 2 & x,0,0 & & (9) & \ 2 & 0,y,0 \\
(2_y | 0,0,0) & & (2_z | 0,0,0) & & (2_y | 0,0,0) \\
(10) & \ c' & (0,0,1/2) \ x,x,z & & (11) & \ c' & (0,0,1/2) \ x,0,z & & (12) & \ c' & (0,0,1/2) \ 0,y,z \\
(m_3 | 0,0,1/2)' & & (m_2 | 0,0,1/2)' & & (m_1 | 0,0,1/2)'
\end{align*}
\]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>i</td>
<td>1 (1) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) y, x-y, z [v, u-v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x + y, x, z [u+v, u, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(5) y, x-y, z+1/2 [v, u-v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6) x + y, x, z+1/2 [u+v, u, w]</td>
</tr>
<tr>
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<td></td>
<td>(7) y, x, z [v, u, w]</td>
</tr>
<tr>
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<td></td>
<td>(8) x-y, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(9) x, x+y, z [u, u+v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y, x+y, z+1/2 [v, u, w]</td>
</tr>
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<td></td>
<td>(11) x-y, y, z+1/2 [u-v, w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) x+y, x+1/2 [u+v, u, w]</td>
</tr>
<tr>
<td>6</td>
<td>h m'..</td>
<td>x, y, 1/4 [u, v, 0]</td>
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<td>y, x, 1/4 [v, u-v, 0]</td>
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<tr>
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<td>x+y, x, 1/4 [u+v, u, 0]</td>
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<td>6</td>
<td>g .2.</td>
<td>x, x, 0 [u, 0, 0]</td>
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<td>x, 2x, 0 [0, u, 0]</td>
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<td>2x, x, 0 [u, u, 0]</td>
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<tr>
<td>4</td>
<td>f 3..</td>
<td>1/3, 2/3, z [0, 0, w]</td>
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<td>1/3, 2/3, z+1/2 [0, 0, w]</td>
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<td></td>
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<td>2/3, 1/3, z [0, 0, w]</td>
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<tr>
<td>4</td>
<td>e 3..</td>
<td>0, 0, z [0, 0, w]</td>
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<td>0, 0, z+1/2 [0, 0, w]</td>
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<td>0, 0, z [0, 0, w]</td>
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<td>0, 0, z+1/2 [0, 0, w]</td>
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<tr>
<td>2</td>
<td>d 6'..</td>
<td>2/3, 1/3, 1/4 [0, 0, 0]</td>
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<td></td>
<td></td>
<td>1/3, 2/3, 3/4 [0, 0, 0]</td>
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<tr>
<td>2</td>
<td>c 6'..</td>
<td>1/3, 2/3, 1/4 [0, 0, 0]</td>
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<td>2/3, 1/3, 3/4 [0, 0, 0]</td>
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<tr>
<td>2</td>
<td>b 6'..</td>
<td>0, 0, 1/4 [0, 0, 0]</td>
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<tr>
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<td></td>
<td>0, 0, 3/4 [0, 0, 0]</td>
</tr>
<tr>
<td>2</td>
<td>a 32.</td>
<td>0, 0, 0 [0, 0, 0]</td>
</tr>
<tr>
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<td>0, 0, 1/2 [0, 0, 0]</td>
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</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p31m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
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</tbody>
</table>

Origin at x,0,0

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p1m'1</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = c/2</td>
<td>b* = b/2</td>
</tr>
</tbody>
</table>

Origin at x,x/2,0
**Origin** on 32'c'

**Asymmetric unit**

- \(0 \leq x \leq 2/3; \ 0 \leq y \leq 2/3; \ 0 \leq z \leq 1/4; \ x \leq (1+y)/2; \ y \leq \min(1-x,(1+x)/2)\)

**Vertices**

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
</tr>
<tr>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
<td>2/3,1/3,1/4</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. \(1\)
2. \(3^* \ 0,0,z (3_z \ 0,0,0)\)
3. \(3^- \ 0,0,z (3_z^- 0,0,0)\)
4. \(m \ x,y,1/4 (m_z 0,0,1/2)\)
5. \(6^- \ 0,0,z; 0,0,1/4 (6_z^- 0,0,1/2)\)
6. \(6^+ \ 0,0,z; 0,0,1/4 (6_z 0,0,1/2)\)
7. \(2' \ x,x,0 (2_y 0,0,0)'\)
8. \(2' \ x,0,0 (2_z 0,0,0)'\)
9. \(2' \ 0,y,0 (2_y 0,0,0)'\)
10. \(c' (0,0,1/2) \ x,x,z (m_y 0,0,1/2)'\)
11. \(c' (0,0,1/2) \ x,0,z (m_z 0,0,1/2)'\)
12. \(c' (0,0,1/2) \ 0,y,z (m_z 0,0,1/2)'\)
Continued

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) ( \bar{y},x-y,z [\bar{v},u-v,w] )</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
<td>(5) ( \bar{y},x-y,z+1/2 [v,u+v,w] )</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,( \bar{z} ) [v,u,w]</td>
<td>(8) x-y,( \bar{y},z ) [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td>(11) x-y,( \bar{y},z+1/2 [u-v,\bar{v},w] )</td>
</tr>
</tbody>
</table>

| 6 h m.. | x,y,1/4 [0,0,w] | \( \bar{y},x-y,1/4 [0,0,w] \) | \( x+y,x,1/4 [0,0,w] \) |
|         | y,x,3/4 [0,0,w] | x-y,\( \bar{y},3/4 [0,0,w] \) | \( \bar{x},x+y,3/4 [0,0,w] \) |

| 6 g .2' | x,\( \bar{x},0 [u,2u,w] \) | x,2x,0 [2\( \bar{u},\bar{u},w \)] | 2x,\( \bar{x},0 [u,u,w] \) |
|         | x,\( \bar{x},1/2 [\bar{u},2\bar{u},w] \) | x,2x,1/2 [2\( \bar{u},u,w \)] | 2x,\( \bar{x},1/2 [\bar{u},u,w] \) |

| 4 f 3.. | \( 1/3,2/3,z [0,0,w] \) | \( 1/3,2/3,z+1/2 [0,0,w] \) | \( 2/3,1/3,z [0,0,w] \) | \( 2/3,1/3,z+1/2 [0,0,w] \) |
| 4 e 3.. | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] |

| 2 d 6.. | \( 2/3,1/3,1/4 [0,0,w] \) | \( 1/3,2/3,3/4 [0,0,w] \) | \( 1/3,2/3,3/4 [0,0,w] \) |
| 2 c 6.. | \( 1/3,2/3,1/4 [0,0,w] \) | \( 2/3,1/3,3/4 [0,0,w] \) | \( 2/3,1/3,3/4 [0,0,w] \) |
| 2 b 6.. | 0,0,1/4 [0,0,w] | 0,0,3/4 [0,0,w] | 0,0,3/4 [0,0,w] |
| 2 a 32' | 0,0,0 [0,0,w] | 0,0,1/2 [0,0,w] | 0,0,1/2 [0,0,w] |

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p31m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a )</td>
<td>( b^* = b )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>p2'mg'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = c )</td>
<td>( b^* = (a + 2b)/2 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [2,1,0]</th>
<th>p1m1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = c/2 )</td>
<td>( b^* = b/2 )</td>
</tr>
</tbody>
</table>

Origin at 0,0,0
**Origin** at center (6/mmm)

**Asymmetric unit**
\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{1+y}{2}; \quad y \leq \frac{x}{2} \]

**Vertices**
- \(0,0,0\)
- \(\frac{1}{2},0,0\)
- \(\frac{2}{3},\frac{1}{3},0\)
- \(0,0,\frac{1}{2}\)
- \(\frac{1}{2},0,\frac{1}{2}\)
- \(\frac{2}{3},\frac{1}{3},\frac{1}{2}\)

**Symmetry Operations**

1. \(1\)
2. \(3^+ (0,0,0)\)
3. \(3^- (0,0,0)\)
4. \(2 \cdot (0,0,z)\)
5. \(2 \cdot (0,0,0)\)
6. \(2 \cdot (0,0,z)\)
7. \(2 \cdot (x,x,0)\)
8. \(2 \cdot (x,0,0)\)
9. \(2 \cdot (0,y,0)\)
10. \(2 \cdot (x,x,0)\)
11. \(2 \cdot (x,2x,0)\)
12. \(2 \cdot (2x,x,0)\)
Continued

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(13) T</td>
<td>0,0,0</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(14) \overline{3}+ 0,0,0; \overline{0},0,0</td>
</tr>
<tr>
<td></td>
<td>(2) \overline{y},x-y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(3) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(15) \overline{3} 0,0,z; 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(3) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>(16) m</td>
<td>x,y,0</td>
</tr>
<tr>
<td></td>
<td>(17) \overline{6} - 0,0,z; 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(2) \overline{y},x-y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(3) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(18) \overline{6} 0,0,z; 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(6) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>(19) m</td>
<td>x,x,z</td>
</tr>
<tr>
<td></td>
<td>(20) m x,2x,z</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(2) \overline{y},x-y,1/2 [0,0,w]</td>
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<tr>
<td></td>
<td>(3) \overline{x}+y,1/2 [0,0,w]</td>
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<tr>
<td></td>
<td>(4) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(6) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(8) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(9) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>(22) m</td>
<td>x,x,z</td>
</tr>
<tr>
<td></td>
<td>(23) m x,0,z</td>
</tr>
<tr>
<td></td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) \overline{y},x-y,1/2 [0,0,w]</td>
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<td>(3) \overline{x}+y,1/2 [0,0,w]</td>
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<td></td>
<td>(4) \overline{x}+y,1/2 [0,0,w]</td>
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<tr>
<td></td>
<td>(5) y,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(6) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(8) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>(9) \overline{x}+y,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>24</td>
<td>r</td>
</tr>
<tr>
<td>1</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>12</td>
<td>q</td>
</tr>
<tr>
<td>m..</td>
<td>x,y,1/2 [0,0,w]</td>
</tr>
<tr>
<td>12</td>
<td>p</td>
</tr>
<tr>
<td>m..</td>
<td>x,y,0 [0,0,w]</td>
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</tbody>
</table>

191.1.1463 - 2 - 3187
<table>
<thead>
<tr>
<th>P6/mmm</th>
<th>191.1.1463</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 o .m.</td>
<td>x,2x,z [u,0,0]</td>
</tr>
<tr>
<td>12 n .m</td>
<td>x,0,z [u,2u,0]</td>
</tr>
<tr>
<td>6 m mm2</td>
<td>x,2x,1/2 [0,0,0]</td>
</tr>
<tr>
<td>6 l mm2</td>
<td>x,2x,0 [0,0,0]</td>
</tr>
<tr>
<td>6 k m2m</td>
<td>x,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>6 j m2m</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>6 i 2mm</td>
<td>1/2,0,z [0,0,0]</td>
</tr>
<tr>
<td>4 h 3m.</td>
<td>1/3,2/3,z [0,0,0]</td>
</tr>
<tr>
<td>3 g mmm</td>
<td>1/2,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 f mmm</td>
<td>1/2,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 e 6mm</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d 6m2</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2 c 6m2</td>
<td>1/3,2/3,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b 6/mmm</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1 a 6/mmm</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p6mm1’
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0] p2mm1’
\[ a^* = c \quad b^* = \frac{(a + 2b)}{2} \]
Origin at x,0,0

Along [2,1,0] p2mm1’
\[ a^* = c \quad b^* = \frac{b}{2} \]
Origin at x,x/2,0
**Origin** at center \((6/mmm1')\)

**Asymmetric unit**

\[
0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq x/2
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2
\end{align*}
\]

**Symmetry Operations**

For \(1 + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 & \quad (2) 3^* & \quad 0,0,z \\
(1 \mid 0,0,0) & \quad (3) 3 & \quad 0,0,z \\
& \quad (3_z \mid 0,0,0) & \quad (3_z^{-1} \mid 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(4) & \quad 2 & \quad 0,0,z \\
\quad (2_z \mid 0,0,0) & \quad (5) 6 & \quad 0,0,z \\
& \quad (6_z^{-1} \mid 0,0,0) & \quad (6_z \mid 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(7) & \quad 2 & \quad x,x,0 \\
\quad (2_{xy} \mid 0,0,0) & \quad (8) 2 & \quad x,0,0 \\
& \quad (2_z \mid 0,0,0) & \quad (2_{y} \mid 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(10) & \quad 2 & \quad x,x,0 \\
\quad (2_z \mid 0,0,0) & \quad (11) 2 & \quad x,2x,0 \\
& \quad (2_{z} \mid 0,0,0) & \quad (2_{z} \mid 0,0,0)
\end{align*}
\]

\[
\begin{align*}
(12) & \quad 2 & \quad 2x,0,0 \\
\quad (2_{z} \mid 0,0,0) & \quad (12) 2 & \quad 2x,0,0 \\
& \quad (2_{z} \mid 0,0,0) & \quad (2_{z} \mid 0,0,0)
\end{align*}
\]
Continued

(13) $\bar{1}$ 0,0,0 \\
    ($\bar{1} | 0,0,0$) \\
(14) $\bar{3}'$ 0,0,z; 0,0,0 \\
    ($3_z | 0,0,0$) \\
(15) $\bar{3}'$ 0,0,z; 0,0,0 \\
    ($3_z^{-1} | 0,0,0$)

(16) m x,y,0 \\
    ($m_x | 0,0,0$) \\
(17) $\bar{6}'$ 0,0,z; 0,0,0 \\
    ($6_z^{-1} | 0,0,0$) \\
(18) $\bar{6}'$ 0,0,z; 0,0,0 \\
    ($6_z | 0,0,0$)

(19) m x,$\bar{x}$,z \\
    ($m_x | 0,0,0$) \\
(20) m x,2x,z \\
    ($m_x | 0,0,0$) \\
(21) m 2x,x,z \\
    ($m_y | 0,0,0$)

(22) m x,x,z \\
    ($m_x | 0,0,0$) \\
(23) m x,0,z \\
    ($m_x | 0,0,0$) \\
(24) m 0,y,z \\
    ($m_x | 0,0,0$)

For 1' + set

(1) 1' \\
    ($1 | 0,0,0$) \\
(2) $3'$ 0,0,z \\
    ($3_z | 0,0,0$)' \\
(3) $3'$ 0,0,z \\
    ($3_z^{-1} | 0,0,0$)'

(4) 2' 0,0,z \\
    ($2_z | 0,0,0$)'

(7) 2' x,x,0 \\
    ($2_y | 0,0,0$)'

(10) 2' x,x,0 \\
    ($2_x | 0,0,0$)'

(13) $\bar{1}'$ \\
    ($\bar{1} | 0,0,0$)' \\
(14) $\bar{3}'$ 0,0,z; 0,0,0 \\
    ($3_z | 0,0,0$)' \\
(15) $\bar{3}'$ 0,0,z; 0,0,0 \\
    ($3_z^{-1} | 0,0,0$)'

(16) m' x,y,0 \\
    ($m_x | 0,0,0$)' \\
(17) $\bar{6}'$ 0,0,z; 0,0,0 \\
    ($6_z^{-1} | 0,0,0$)' \\
(18) $\bar{6}'$ 0,0,z; 0,0,0 \\
    ($6_z | 0,0,0$)'

(19) m' x,$\bar{x}$,z \\
    ($m_x | 0,0,0$)'

(22) m' x,x,z \\
    ($m_x | 0,0,0$)'

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

<table>
<thead>
<tr>
<th>1 +</th>
<th>1' +</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 r 11'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) $\bar{x}$,$\bar{y}$,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(10) $\bar{y}$,$\bar{x}$,z [0,0,0]</td>
</tr>
</tbody>
</table>
Continued 191.2.1464 P6/mmm1'

(13) $x, y, z [0,0,0]$
(14) $y, x+y, z [0,0,0]$
(15) $x-y, x, z [0,0,0]$

(16) $x, y, z [0,0,0]$
(17) $y, x-y, z [0,0,0]$
(18) $x+y, x, z [0,0,0]$

(19) $y, x, z [0,0,0]$
(20) $x+y, y, z [0,0,0]$
(21) $x, x-y, z [0,0,0]$

(22) $y, x, z [0,0,0]$
(23) $x-y, y, z [0,0,0]$
(24) $x, x+y, z [0,0,0]$

12 $q \ m..1'$

$x, y, 1/2 [0,0,0]$
$y, x-y, 1/2 [0,0,0]$
$x+y, x, 1/2 [0,0,0]$

$x, y, 1/2 [0,0,0]$
$y, x+y, 1/2 [0,0,0]$
$x-y, x, 1/2 [0,0,0]$

$y, x, 1/2 [0,0,0]$
$y+x, y, 1/2 [0,0,0]$
$x+y, x, 1/2 [0,0,0]$

12 $p \ m..1'$

$x, y, 0 [0,0,0]$
$y, x-y, 0 [0,0,0]$
$x+y, x, 0 [0,0,0]$

$x, y, 0 [0,0,0]$
$y, x+y, 0 [0,0,0]$
$x-y, x, 0 [0,0,0]$

$y, x, 0 [0,0,0]$
$x+y, y, 0 [0,0,0]$
$x, x-y, 0 [0,0,0]$

12 $o \ m..1'$

$x, 2x, z [0,0,0]$
$2x, x, z [0,0,0]$
$x, x, z [0,0,0]$

$x, 2x, z [0,0,0]$
$2x, x, z [0,0,0]$
$x, x, z [0,0,0]$

$2x, x, z [0,0,0]$
$x, 2x, z [0,0,0]$
$x, x, z [0,0,0]$

12 $n \ m..1'$

$x, 0, z [0,0,0]$
$0, x, z [0,0,0]$
$x, x, z [0,0,0]$

$x, 0, z [0,0,0]$
$0, x, z [0,0,0]$
$x, x, z [0,0,0]$

$0, x, z [0,0,0]$
$x, 0, z [0,0,0]$
$x, x, z [0,0,0]$

6 $m \ mm21'$

$x, 2x, 1/2 [0,0,0]$
$2x, x, 1/2 [0,0,0]$
$x, x, 1/2 [0,0,0]$

$x, 2x, 1/2 [0,0,0]$
$2x, x, 1/2 [0,0,0]$
$x, x, 1/2 [0,0,0]$

6 $l \ mm21'$

$x, 2x, 0 [0,0,0]$
$2x, x, 0 [0,0,0]$
$x, x, 0 [0,0,0]$

$x, 2x, 0 [0,0,0]$
$2x, x, 0 [0,0,0]$
$x, x, 0 [0,0,0]$

6 $k \ m2m1'$

$x, 0, 1/2 [0,0,0]$
$0, x, 1/2 [0,0,0]$
$x, x, 1/2 [0,0,0]$

$x, 0, 1/2 [0,0,0]$
$0, x, 1/2 [0,0,0]$
$x, x, 1/2 [0,0,0]$

6 $j \ m2m1'$

$x, 0, 0 [0,0,0]$
$0, x, 0 [0,0,0]$
$x, x, 0 [0,0,0]$

$x, 0, 0 [0,0,0]$
$0, x, 0 [0,0,0]$
$x, x, 0 [0,0,0]$

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6  i  2mm1'  1/2,0,z [0,0,0]  0,1/2,z [0,0,0]  1/2,1/2,z [0,0,0]
   0,1/2,z [0,0,0]  1/2,0,z [0,0,0]  1/2,1/2,z [0,0,0]
4  h  3m.1'  1/3,2/3,z [0,0,0]  2/3,1/3,z [0,0,0]  2/3,1/3,z [0,0,0]  1/3,2/3,z [0,0,0]
3  g  mmm1'  1/2,0,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]
3  f  mmm1'  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]
2  e  6mm1'  0,0,z [0,0,0]  0,0,z [0,0,0]
2  d  6m21'  1/3,2/3,1/2 [0,0,0]  2/3,1/3,1/2 [0,0,0]
2  c  6m21'  1/3,2/3,0 [0,0,0]  2/3,1/3,0 [0,0,0]
1  b  6/mmm1'  0,0,1/2 [0,0,0]
1  a  6/mmm1'  0,0,0 [0,0,0]

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mm1'</th>
<th>Along [2,1,0]</th>
<th>p2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = c</td>
<td>b* = (a + 2b)/2</td>
<td>a* = c</td>
<td>b* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at center (6/m\'mm)

**Asymmetric unit**

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \frac{x}{2} \]

**Vertices**

\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2
\end{align*}

**Symmetry Operations**

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^- \quad 0,0,z \\
(4) & \quad 2 \quad 0,0,z \\
(5) & \quad 6^* \quad 0,0,z \\
(6) & \quad 6^- \quad 0,0,z \\
(7) & \quad 2' \quad x,x,0 \\
(8) & \quad 2' \quad x,0,0 \\
(9) & \quad 2' \quad 0,y,0 \\
(10) & \quad 2' \quad x,x,0 \\
(11) & \quad 2' \quad x,2x,0 \\
(12) & \quad 2' \quad 2x,0,0 \\
\end{align*}
Continued

191.3.1465

P6/m'mm

(13) \( \bar{1} \) | 0,0,0
(14) \( \bar{3} \) | 0,0,0
(15) \( \bar{3} \) | 0,0,0
(16) \( \bar{m} \) | x,y,0
(17) \( \bar{6} \) | 0,0,0
(18) \( \bar{6} \) | 0,0,0
(19) \( \bar{m} \) | x,z
(20) \( \bar{m} \) | x,2x,z
(21) \( \bar{m} \) | 2x,x,z
(22) \( \bar{m} \) | x,z
(23) \( \bar{m} \) | x,0,z
(24) \( \bar{m} \) | 0,y,z

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 r 1</td>
<td>(1) x,y,z [u,v,w] (2) ( \bar{y} \cdot x\cdot y\cdot \bar{z} [\bar{v} \cdot u\cdot v\cdot w] ) (3) ( x\cdot y\cdot \bar{z} [\bar{u} + v\cdot \bar{u}\cdot w] )</td>
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<td>(4) ( x\cdot \bar{y}\cdot z [\bar{u} \cdot \bar{v} \cdot w] ) (5) y,x+y,z [v,u+v,w] (6) x-y,x,z [u-v,u,w]</td>
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</tbody>
</table>
|              | (7) y,x,z [v,u,w] (8) x-y,\( \bar{y}\cdot \bar{z} [\bar{u} \cdot v\cdot w] \) (9) x,\( \bar{x} + y\cdot z \cdot [u\cdot u\cdot v\cdot w] \)
|              | (10) y,\( x\cdot \bar{z} [v\cdot u\cdot w] \) (11) \( x + y\cdot \bar{z} [\bar{u} \cdot v\cdot w] \) (12) x-x,y,z [\( u\cdot u\cdot v\cdot w \) |
|              | (13) \( \bar{x}\cdot \bar{y}\cdot \bar{z} [\bar{u} \cdot \bar{v}\cdot w] \) (14) y,\( \bar{x} + y\cdot \bar{z} [\bar{v} \cdot u\cdot v\cdot w] \) (15) x-y,x,z [\( u\cdot u\cdot v\cdot w \) |
|              | (16) x,y,z [v,u,w] (17) \( \bar{x}\cdot \bar{x}\cdot z [\bar{v} \cdot u\cdot v\cdot w] \) (18) \( x + y\cdot x\cdot z \cdot [u\cdot v\cdot w] \)
|              | (19) \( \bar{y}\cdot \bar{x}\cdot z [v\cdot u\cdot w] \) (20) \( x + y\cdot y\cdot z \cdot [u\cdot v\cdot \bar{w}] \) (21) x-x,y,z [\( u\cdot u\cdot v\cdot w \) |
|              | (22) \( y\cdot x\cdot z [v\cdot u\cdot w] \) (23) x-y,y,z [\( u\cdot u\cdot v\cdot w \) (24) \( \bar{x}\cdot x\cdot y\cdot z [u\cdot u\cdot v\cdot w] \)

12 q \( m'\cdot \)

<p>| 12 p ( m'\cdot ) |
|---------------------|-------------------|
| x,y,1/2 [u,v,0]    | ( \bar{y}\cdot x\cdot y\cdot 1/2 [\bar{v}\cdot u\cdot v\cdot 0] ) |
| x,y,1/2 [u,\bar{v},0] | y\cdot x\cdot y\cdot 1/2 [v\cdot \bar{u}\cdot v\cdot 0] |
| y,x,1/2 [\bar{v},u,0] | x-y\cdot y\cdot 1/2 [\bar{u}\cdot v\cdot v\cdot 0] |
| y,y,1/2 [v,u,0]    | ( \bar{x}\cdot \bar{y}\cdot 1/2 [v\cdot v\cdot \bar{w}] ) |
| x,y,0 [u,v,0]      | ( y\cdot x\cdot y\cdot 0 [\bar{v}\cdot u\cdot v\cdot 0] ) |
| x,y,0 [u,\bar{v},0] | y\cdot x\cdot y\cdot 0 [v\cdot \bar{u}\cdot v\cdot 0] |
| y,x,0 [\bar{v},u,0] | x\cdot x\cdot y\cdot 0 [u\cdot \bar{u}\cdot v\cdot 0] |
| y,y,0 [v,u,0]      | ( x\cdot x\cdot 0 [u\cdot u\cdot v\cdot 0] ) |
| y,y,0 [v,\bar{u},0] | ( x\cdot x\cdot 0 [u\cdot \bar{u}\cdot v\cdot 0] ) |</p>
<table>
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<tr>
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<tbody>
<tr>
<td>12</td>
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<td>j</td>
<td>m'2'm</td>
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<td>6</td>
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<td>h</td>
<td>3m.</td>
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<td>g</td>
<td>m'mm</td>
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<td>f</td>
<td>m'mm</td>
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<td>e</td>
<td>6mm</td>
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<tr>
<td>2</td>
<td>d</td>
<td>6'm2'</td>
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<tr>
<td>2</td>
<td>c</td>
<td>6'm2'</td>
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<td>1</td>
<td>b</td>
<td>6/m'mm</td>
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<tr>
<td>1</td>
<td>a</td>
<td>6/m'mm</td>
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</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p6mm  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \)  
Origin at x,0,0

Along [2,1,0] p2mm1'  
\( \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2 \)  
Origin at x,x/2,0
**Origin** at center \((6'/mm'm)\)

**Asymmetric unit**

- \(0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq x/2\)

**Vertices**

- \((0,0,0)\)
- \((1/2,0,0)\)
- \((2/3,1/3,0)\)
- \((0,0,1/2)\)
- \((1/2,0,1/2)\)
- \((2/3,1/3,1/2)\)

**Symmetry Operations**

1. \(1\)
2. \(3' \quad 0,0,z\)
3. \(3' \quad 0,0,z\)
4. \(2' \quad 0,0,z\)
5. \(6' \quad 0,0,z\)
6. \(6' \quad 0,0,z\)
7. \(2 \quad x,x,0\)
8. \(2 \quad x,0,0\)
9. \(2 \quad 0,y,0\)
10. \(2' \quad x,x,0\)
11. \(2' \quad x,2x,0\)
12. \(2' \quad 2x,x,0\)

(1) \(1\)
(1) \(0,0,0\)

(2) \(3' \quad 0,0,z\)
(3) \(3' \quad 0,0,z\)

(4) \(2' \quad 0,0,z\)
(5) \(6' \quad 0,0,z\)
(6) \(6' \quad 0,0,z\)

(7) \(2 \quad x,x,0\)
(8) \(2 \quad x,0,0\)
(9) \(2 \quad 0,y,0\)

(10) \(2' \quad x,x,0\)
(11) \(2' \quad x,2x,0\)
(12) \(2' \quad 2x,x,0\)
Continued

(13) \( \overline{1}^* \), 0,0,0
(14) \( \overline{3}^* \), 0,0,0
(15) \( \overline{3}^* \), 0,0

(16) m \( x,y,0 \)
(17) \( \overline{6} \), 0,0,0
(18) \( \overline{6} \), 0,0,0

(19) m' \( x,x,z \)
(20) m' \( x,2x,z \)
(21) m' \( 2x,x,z \)

(22) m \( x,x,z \)
(23) m \( x,0,z \)
(24) m \( 0,y,z \)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

24 r 1
(1) \( x,y,z \) [u,v,w]
(2) \( \overline{y},x-y,z \) [\( \overline{v},u-v,w \)]
(3) \( \overline{x}+y,x,z \) [\( \overline{u}+v,u,w \)]

(4) \( \overline{x},\overline{y},z \) [u,v,w]
(5) \( y,\overline{x}+y,z \) [\( \overline{v},u-v,w \)]
(6) \( x-y,x,z \) [\( u-v,u,w \)]

(7) y,x,z [v,u,w]
(8) x-y,\( \overline{y},z \) [\( u-v,\overline{v},w \)]
(9) x,\( \overline{x}+y,z \) [\( \overline{u},u+v,w \)]

(10) \( \overline{y},x-z \) [v,u,w]
(11) \( \overline{x}+y,\overline{z} \) [u-v,\( \overline{v},w \)]
(12) \( \overline{x},x,\overline{z} \) [\( \overline{u},u+v,w \)]

(13) \( \overline{x},\overline{y},z \) [u,v,w]
(14) \( y,\overline{x}+y,z \) [\( v,\overline{u}+v,w \)]
(15) \( x+y,\overline{x},z \) [\( u-v,\overline{u},w \)]

(16) x,y,z [u,v,w]
(17) \( \overline{y},\overline{x}+y,z \) [\( v,\overline{u}+v,w \)]
(18) \( \overline{x}+y,\overline{x},z \) [\( u-v,\overline{u},w \)]

(19) \( y,\overline{x},z \) [\( \overline{v},\overline{u},w \)]
(20) \( \overline{x}+y,y,z \) [\( \overline{u}+v,v,w \)]
(21) \( x-x,y,z \) [\( u-u-v,w \)]

(22) y,x,z [v,u,w]
(23) \( \overline{y},\overline{x},z \) [\( \overline{u}+v,v,w \)]
(24) \( \overline{x},\overline{x},y,z \) [\( u-u-v,w \)]

12 q m.. x,y,1/2 [0,0,w]
\( \overline{y},x-y,1/2 \) [0,0,w]
\( \overline{x},x-1/2 \) [0,0,w]

12 p m.. x,y,0 [0,0,w]
\( \overline{y},x-y,0 \) [0,0,w]
\( \overline{x},x,0 \) [0,0,w]
| 12 | o   | m'  | x,2x,z [u,2u,w] | 2x,x,z [2u, u,w] | x,x,z [u,u,w] |
|    |     |     |                |                |                |
|    |     |     | x,2x,z [u,2u,w] | 2x,x,z [2u, u,w] | x,x,z [u,u,w] |
|    |     |     | 2x,x,z [u,2u,w] | x,2x,z [u,2u,w] | x,x,z [u,u,w] |
|    |     |     | 2x,x,z [2u,u,w] | x,2x,z [u,2u,w] | x,x,z [u,u,w] |
| 12 | n   | m   | x,0,z [u,2u,0] | 0,x,z [2u, u,0] | x,x,z [u,u,0] |
|    |     |     | x,0,z [u,2u,0] | 0,x,z [2u, u,0] | x,x,z [u,u,0] |
|    |     |     | 0,x,z [2u,u,0] | x,0,z [u,2u,0] | x,x,z [u,u,0] |
|    |     |     | 0,x,z [2u,u,0] | x,0,z [u,2u,0] | x,x,z [u,u,0] |
| 6  | m   | mm'2' | x,2x,1/2 [0,0,w] | 2x,x,1/2 [0,0,w] | x,x,1/2 [0,0,w] |
|    |     |     | x,2x,1/2 [0,0,w] | 2x,x,1/2 [0,0,w] | x,x,1/2 [0,0,w] |
| 6  | l   | mm'2' | x,2x,0 [0,0,w] | 2x,x,0 [0,0,w] | x,x,0 [0,0,w] |
|    |     |     | x,2x,0 [0,0,w] | 2x,x,0 [0,0,w] | x,x,0 [0,0,w] |
| 6  | k   | m2m  | x,0,1/2 [0,0,0] | 0,x,1/2 [0,0,0] | x,x,1/2 [0,0,0] |
|    |     |     | x,0,1/2 [0,0,0] | 0,x,1/2 [0,0,0] | x,x,1/2 [0,0,0] |
| 6  | j   | m2m  | x,0,0 [0,0,0] | 0,x,0 [0,0,0] | x,x,0 [0,0,0] |
|    |     |     | x,0,0 [0,0,0] | 0,x,0 [0,0,0] | x,x,0 [0,0,0] |
| 6  | i   | 2'm'm | 1/2,0,z [u,2u,0] | 0,1/2,z [2u, u,0] | 1/2,1/2,z [u,u,0] |
|    |     |     | 0,1/2,z [u,2u,0] | 1/2,0,z [2u, u,0] | 1/2,1/2,z [u,u,0] |
| 4  | h   | 3m'  | 1/3,2/3,z [0,0,w] | 2/3,1/3,z [0,0,w] | 1/3,2/3,z [0,0,w] |
| 3  | g   | mm'm  | 1/2,0,1/2 [0,0,0] | 0,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |
| 3  | f   | mm'm  | 1/2,0,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 2  | e   | 6'm'm  | 0,0,z [0,0,0] | 0,0,z [0,0,0] | |
| 2  | d   | 6'm'2' | 1/3,2/3,1/2 [0,0,w] | 2/3,1/3,1/2 [0,0,w] | |
| 2  | c   | 6'm'2' | 1/3,2/3,0 [0,0,w] | 2/3,1/3,0 [0,0,w] | |
| 1  | b   | 6'1/m'm  | 0,0,1/2 [0,0,0] | |
| 1  | a   | 6'1/m'm  | 0,0,0 [0,0,0] | |
Symmetry of Special Projections

Along \([0,0,1]\) \(p6mm1'\)
- \(a^* = a\)
- \(b^* = b\)
- Origin at \(0,0,z\)

Along \([1,0,0]\) \(p2mm\)
- \(a^* = c\)
- \(b^* = (\mathbf{a} + 2\mathbf{b})/2\)
- Origin at \(x,0,0\)

Along \([2,1,0]\) \(p2mm1'\)
- \(a^* = c\)
- \(b^* = b/2\)
- Origin at \(x,x/2,0\)
Origin at center (6'/mmm')

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq (1+y)/2; \quad y \leq x/2 \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^* \quad 0,0,z \\
(4) & \quad 2' \quad 0,0,z \\
(2_{\pi}) & \quad 0,0,0)' \\
(5) & \quad 6' \quad 0,0,z \\
(6) & \quad 6' \quad 0,0,z \\
(7) & \quad 2' \quad x,x,0 \\
(2_{\pi}) & \quad 0,0,0)' \\
(8) & \quad 2' \quad x,0,0 \\
(2_{\pi}) & \quad 0,0,0)' \\
(9) & \quad 9' \quad 0,y,0 \\
(2_{\pi}) & \quad 0,0,0)' \\
(10) & \quad 2 \quad x,x,0 \\
(2_{\pi}) & \quad 0,0,0) \\
(11) & \quad 2 \quad x,2x,0 \\
(2_{\pi}) & \quad 0,0,0) \\
(12) & \quad 2 \quad 2x,x,0 \\
(2_{\pi}) & \quad 0,0,0)
\end{align*}
\]
Continued

(13) $\overline{1}$' 0,0,0
($\overline{1} | 0,0,0 \rangle$)

(14) $\overline{3}^{+}$' 0,0,z; 0,0,0
($3_{z}^{+} | 0,0,0 \rangle$)

(15) $\overline{3}^{-}$' 0,0,z; 0,0,0
($3_{z}^{-} | 0,0,0 \rangle$)

(16) m x,y,0
($m_{x} | 0,0,0 \rangle$)

(17) $\overline{6}^{-}$ 0,0,z; 0,0,0
($\overline{6}_{z}^{-} | 0,0,0 \rangle$)

(18) $\overline{6}^{-}$ 0,0,z; 0,0,0
($\overline{6}_{z}^{-} | 0,0,0 \rangle$)

(19) m x,\overline{x},z
($m_{x} | 0,0,0 \rangle$)

(20) m x,2x,z
($m_{x} | 0,0,0 \rangle$)

(21) m 2x,x,z
($m_{y} | 0,0,0 \rangle$)

(22) m' x,x,z
($m_{x} | 0,0,0 \rangle$)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 r 1
(1) x,y,z [u,v,w]
(2) y,x-y,z [v,u-v,w]
(3) x+y,x,z [u+v,u,w]
(4) x,y,z [u,v,w]
(5) y,x+y,z [v,u-v,w]
(6) x-y,x,z [u-v,u,w]
(7) y,x,z [v,u,w]
(8) x-y,y,z [v,u-v,w]
(9) x,x+y,z [u,u-v,w]
(10) y,x,z [v,u,w]
(11) x+y,x,z [u+v,u,w]
(12) x,x+y,z [u,u-v,w]
(13) x,y,z [u,v,w]
(14) y,x+y,z [v,u-v,w]
(15) x-y,x,z [u-v,u,w]
(16) x,y,z [u,v,w]
(17) y,x+y,z [v,u-v,w]
(18) x-y,x,z [u-v,u,w]
(19) y,x,z [v,u,w]
(20) x+y,x,z [u+v,u,w]
(21) x,x+y,z [u,u+v,w]
(22) y,x,z [v,u,w]
(23) x-y,y,z [u-v,v,w]
(24) x+y,x,z [u,u+v,w]

12 q m.. x,y,1/2 [0,0,w]
$\overline{y}$,x-y,1/2 [0,0,w]
$\overline{x}$,y,1/2 [0,0,w]
y,x+y,1/2 [0,0,w]
$x$,y,1/2 [0,0,w]
y,x,1/2 [0,0,w]
$x$,y,1/2 [0,0,w]
$\overline{y}$,x,1/2 [0,0,w]
x+y,y,1/2 [0,0,w]
$\overline{x}$,x+y,1/2 [0,0,w]
x,y,1/2 [0,0,w]

12 p m.. x,y,0 [0,0,w]
$\overline{y}$,x-y,0 [0,0,w]
$\overline{x}$,y,0 [0,0,w]
y,x+y,0 [0,0,w]
y,x,0 [0,0,w]
x-y,$\overline{y}$,0 [0,0,w]
y,$\overline{y}$,0 [0,0,w]
y,x,0 [0,0,w]
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<th>No.</th>
<th>Symbol</th>
<th>Description</th>
<th>191.5.1467</th>
<th>P6'/mmm'</th>
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<td>12 o</td>
<td>m.</td>
<td>x,2x,z [u,0,0]</td>
<td>2x,x,z [0,u,0]</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,z [u,0,0]</td>
<td>2x,x,z [0,u,0]</td>
<td>x,x,z [u,u,0]</td>
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<td>2x,x,z [u,0,0]</td>
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<tr>
<td>12 n</td>
<td>.m</td>
<td>x,0,z [u,0,w]</td>
<td>0,x,z [0,u,w]</td>
<td>x,x,z [u,u,w]</td>
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<td>x,0,z [u,0,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>x,0,z [u,0,w]</td>
<td>x,x,z [u,u,w]</td>
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<tr>
<td>6 m</td>
<td>mm2</td>
<td>x,2x,1/2 [0,0,0]</td>
<td>2x,x,1/2 [0,0,0]</td>
<td>x,x,1/2 [0,0,0]</td>
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<tr>
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<td>x,2x,1/2 [0,0,0]</td>
<td>2x,x,1/2 [0,0,0]</td>
<td>x,x,1/2 [0,0,0]</td>
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<tr>
<td>6 l</td>
<td>mm2</td>
<td>x,2x,0 [0,0,0]</td>
<td>2x,x,0 [0,0,0]</td>
<td>x,x,0 [0,0,0]</td>
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<td>x,2x,0 [0,0,0]</td>
<td>2x,x,0 [0,0,0]</td>
<td>x,x,0 [0,0,0]</td>
</tr>
<tr>
<td>6 k</td>
<td>m2'm'</td>
<td>x,0,1/2 [0,0,w]</td>
<td>0,x,1/2 [0,0,w]</td>
<td>x,x,1/2 [0,0,w]</td>
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<tr>
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<td>x,0,1/2 [0,0,w]</td>
<td>0,x,1/2 [0,0,w]</td>
<td>x,x,1/2 [0,0,w]</td>
</tr>
<tr>
<td>6 j</td>
<td>m2'm'</td>
<td>x,0,0 [0,0,w]</td>
<td>0,x,0 [0,0,w]</td>
<td>x,x,0 [0,0,w]</td>
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<tr>
<td></td>
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<td>x,0,0 [0,0,w]</td>
<td>0,x,0 [0,0,w]</td>
<td>x,x,0 [0,0,w]</td>
</tr>
<tr>
<td>6 i</td>
<td>2'mm'</td>
<td>1/2,0,z [u,0,0]</td>
<td>0,1/2,z [u,0,0]</td>
<td>1/2,1/2,z [u,u,0]</td>
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<td>0,1/2,z [u,0,0]</td>
<td>1/2,0,z [u,0,0]</td>
<td>1/2,1/2,z [u,u,0]</td>
</tr>
<tr>
<td>4 h</td>
<td>3m.</td>
<td>1/3,2/3,z [0,0,0]</td>
<td>2/3,1/3,z [0,0,0]</td>
<td>2/3,1/3,z [0,0,0]</td>
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<td>1/3,2/3,z [0,0,0]</td>
<td>2/3,1/3,z [0,0,0]</td>
<td>1/3,2/3,z [0,0,0]</td>
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<tr>
<td>3 g</td>
<td>mmm'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3 f</td>
<td>mmm'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>2 e</td>
<td>6'mm'</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
</tr>
<tr>
<td>2 d</td>
<td>6m2</td>
<td>1/3,2,3,1/2 [0,0,0]</td>
<td>2/3,1,3,1/2 [0,0,0]</td>
<td>2/3,1,3,1/2 [0,0,0]</td>
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<tr>
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<td>6m2</td>
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<td>2/3,1,3,0 [0,0,0]</td>
<td>2/3,1,3,0 [0,0,0]</td>
</tr>
<tr>
<td>1 b</td>
<td>6'mmm'</td>
<td>0,0,1/2 [0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>1 a</td>
<td>6'mmm'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Symmetry</th>
<th>Relations</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1] p6mm'</td>
<td>$\mathbf{a}^* = \mathbf{a}$ $\mathbf{b}^* = \mathbf{b}$</td>
<td></td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Along [1,0,0] p2mm'</td>
<td>$\mathbf{a}^* = \mathbf{c}$ $\mathbf{b}^* = (\mathbf{a} + \mathbf{2b})/2$</td>
<td></td>
<td>Origin at x,0,0</td>
</tr>
<tr>
<td>Along [2,1,0] p2mm</td>
<td>$\mathbf{a}^* = \mathbf{c}$ $\mathbf{b}^* = \mathbf{b}/2$</td>
<td></td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
**Origin** at center (6/m'm'm)

**Asymmetric unit**

- \(0 \leq x \leq 2/3;\) \(0 \leq y \leq 1/3;\) \(0 \leq z \leq 1/2;\) \(x \leq (1+y)/2;\) \(y \leq x/2\)

**Vertices**
- \((0,0,0)\)
- \((1/2,0,0)\)
- \((2/3,1/3,0)\)
- \((0,0,1/2)\)
- \((1/2,0,1/2)\)
- \((2/3,1/3,1/2)\)

**Symmetry Operations**

- (1) \(1\)
- (2) \(3^* \ 0,0,z\)
- (3) \(3' \ 0,0,z\)
- (4) \(2' \ 0,0,z\)
- (5) \(6' \ 0,0,z\)
- (6) \(6'' \ 0,0,z\)
- (7) \(2' \ x,x,0\)
- (8) \(2' \ x,0,0\)
- (9) \(2' \ 0,y,0\)
- (10) \(2 \ x,x,0\)
- (11) \(2 \ x,2x,0\)
- (12) \(2 \ 2x,0\)
Continued 191.6.1468 P6'/m'm'm

<table>
<thead>
<tr>
<th>(13)</th>
<th>0,0,0</th>
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<tbody>
<tr>
<td>(14)</td>
<td>0,0,z; 0,0,0</td>
</tr>
<tr>
<td>(15)</td>
<td>0,0,z; 0,0,0</td>
</tr>
<tr>
<td>(16)</td>
<td>m' x,y,0</td>
</tr>
<tr>
<td>(17)</td>
<td>0,0,z; 0,0,0</td>
</tr>
<tr>
<td>(18)</td>
<td>0,0,z; 0,0,0</td>
</tr>
<tr>
<td>(19)</td>
<td>m' x,x,z</td>
</tr>
<tr>
<td>(20)</td>
<td>m' x,2x,z</td>
</tr>
<tr>
<td>(21)</td>
<td>m' 2x,x,z</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

<table>
<thead>
<tr>
<th>Positions</th>
</tr>
</thead>
</table>

| Multiplicity, Wyckoff letter, Site Symmetry. |

<table>
<thead>
<tr>
<th>Coordinates</th>
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**Positions**

<table>
<thead>
<tr>
<th>24 r 1</th>
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<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<tr>
<td>(4) x,y,z [u,v,w]</td>
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<tr>
<td>(5) y,x+y,z [v,u-v,w]</td>
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<tr>
<td>(6) x+y,x,z [u+v,u,w]</td>
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<tr>
<td>(7) y,x,z [v,u-w]</td>
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<td>(8) x-y,y,z [u+v,v,w]</td>
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<tr>
<td>(9) x,x+y,z [u,u-v,w]</td>
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<td>(10) y,x,z [v,u-w]</td>
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<tr>
<td>(11) x+y,y,z [u+v,v,w]</td>
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<tr>
<td>(12) x,x+y,z [u,u-v,w]</td>
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<tr>
<td>(13) x,y,z [v,u-w]</td>
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<tr>
<td>(14) y,x+y,z [v,u-v,w]</td>
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<tr>
<td>(15) x+y,x,z [u+v,u,w]</td>
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<tr>
<td>(16) x,y,z [v,u-w]</td>
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<tr>
<td>(17) y,x+y,z [v,u-v,w]</td>
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<tr>
<td>(18) x+y,x,z [u+v,u,w]</td>
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<tr>
<td>(19) y,x,z [v,u-w]</td>
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<tr>
<td>(20) x+y,y,z [u+v,v,w]</td>
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<tr>
<td>(21) x,x+y,z [u,u-v,w]</td>
</tr>
<tr>
<td>(22) y,x,z [v,u-w]</td>
</tr>
<tr>
<td>(23) x-y,y,z [u+v,v,w]</td>
</tr>
<tr>
<td>(24) x,x+y,z [u,u-v,w]</td>
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</table>

<table>
<thead>
<tr>
<th>12 q m'.</th>
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<tbody>
<tr>
<td>x,y,1/2 [u,v,0]</td>
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<tr>
<td>y,x-y,1/2 [v,u-v,0]</td>
</tr>
<tr>
<td>x+y,x,1/2 [u+v,u,0]</td>
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<tr>
<td>x,y,1/2 [u,v,0]</td>
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<tr>
<td>y,x+y,1/2 [v,u-v,0]</td>
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<td>x+y,x,1/2 [u+v,u,0]</td>
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<tr>
<td>y,x,1/2 [v,u,0]</td>
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<tr>
<td>x+y,y,1/2 [u+v,v,0]</td>
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<tr>
<td>x,x+y,1/2 [u,u-v,0]</td>
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<tbody>
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<td>x,y,0 [u,v,0]</td>
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<tr>
<td>y,x-y,0 [v,u-v,0]</td>
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<tr>
<td>x+y,x,0 [u+v,u,0]</td>
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<tr>
<td>x,y,0 [u,v,0]</td>
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<tr>
<td>y,x+y,0 [v,u-v,0]</td>
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<tr>
<td>x+y,x,0 [u+v,u,0]</td>
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<td>x,x+y,0 [u,u-v,0]</td>
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</table>
Symmetry of Special Projections

Along \([0,0,1]\)  \(p6'm'm\)
\[
\begin{align*}
\mathbf{a}^* &= \mathbf{a} & \mathbf{b}^* &= \mathbf{b} \\
\text{Origin at } 0,0,z
\end{align*}
\]

Along \([1,0,0]\)  \(p2'mm'\)
\[
\begin{align*}
\mathbf{a}^* &= (\mathbf{a} + 2\mathbf{b})/2 & \mathbf{b}^* &= \mathbf{c} \\
\text{Origin at } x,0,0
\end{align*}
\]

Along \([2,1,0]\)  \(p2mm1'\)
\[
\begin{align*}
\mathbf{a}^* &= \mathbf{c} & \mathbf{b}^* &= \mathbf{b}/2 \\
\text{Origin at } x,x/2,0
\end{align*}
\]
Origin at center (6/m/mm')

Asymmetric unit

\[0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq x/2\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \quad 0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2\]

Symmetry Operations

1. \(1\)
   \(1|0,0,0\)

2. \(3^+\)
   \(0,0,z\)
   \(3_z|0,0,0\)

3. \(3^-\)
   \(0,0,z\)
   \(3_z^{-1}|0,0,0\)

4. \(2'\)
   \(0,0,z\)
   \(2_z|0,0,0\)

5. \(6'\)
   \(0,0,z\)
   \(6_z|0,0,0\)

6. \(6''\)
   \(0,0,z\)
   \(6_z^{-1}|0,0,0\)

7. \(2\)
   \(x,x,0\)
   \(2_{xy}|0,0,0\)

8. \(2\)
   \(x,0,0\)
   \(2_{x}|0,0,0\)

9. \(2\)
   \(0,y,0\)
   \(2_{y}|0,0,0\)

10. \(2'\)
    \(x,x,0\)
    \(2_{z}|0,0,0\)

11. \(2'\)
    \(x,2x,0\)
    \(2_{z}|0,0,0\)

12. \(2'\)
    \(2x,x,0\)
    \(2_{z}|0,0,0\)
Generators selected

(13) \[ \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \]
(14) \[ \begin{pmatrix} 0 & 0 & z \\ 0 & 0 & 0 \\ 3 & z & 1 \end{pmatrix} \]
(15) \[ \begin{pmatrix} 0 & 0 & z \\ 0 & 0 & 0 \\ 3 & z & 1 \end{pmatrix} \]

(16) \[ \begin{pmatrix} m' & x & y \\ 0 & 0 & 0 \end{pmatrix} \]
(17) \[ \begin{pmatrix} 6 & - & 0 \\ 0 & 0 & 0 \end{pmatrix} \]
(18) \[ \begin{pmatrix} 6 & - & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

(19) \[ \begin{pmatrix} m & x & x \\ 0 & 0 & 0 \end{pmatrix} \]
(20) \[ \begin{pmatrix} m & x & 2x \\ 0 & 0 & 0 \end{pmatrix} \]
(21) \[ \begin{pmatrix} m & 2x & x \\ 0 & 0 & 0 \end{pmatrix} \]

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).
| 12 | o | .m. | x,2x,z [u,0,0] | 2x, x,z [0,u,0] | x,x,z [u,u,0] |
| 12 | n | .m' | x,0,z [u,0,w] | 0,x,z [0,u,w] | x,x,z [u,u,w] |
| 6  | m | m'm2' | x,2x,1/2 [u,0,0] | 2x, x,1/2 [0,u,0] | x,x,1/2 [u,u,0] |
| 6  | l | m'm2' | x,2x,0 [u,0,0] | 2x, x,0 [0,u,0] | x,x,0 [u,u,0] |
| 6  | k | m'2m' | x,0,1/2 [u,0,0] | 0,x,1/2 [0,u,0] | x,x,1/2 [u,u,0] |
| 6  | j | m'2m' | x,0,0 [u,0,0] | 0,x,0 [0,u,0] | x,x,0 [u,u,0] |
| 6  | i | 2'mm' | 1/2,0,z [u,0,0] | 0,1/2,z [0,u,0] | 1/2,1/2,z [u,u,0] |
| 4  | h | 3m. | 1/3,2/3,z [0,0,0] | 2/3,1/3,z [0,0,0] | 2/3,1/3,z [0,0,0] |
| 3  | g | m'mm' | 1/2,0,1/2 [u,0,0] | 0,1/2,1/2 [0,u,0] | 1/2,1/2,1/2 [u,u,0] |
| 3  | f | m'mm' | 1/2,0,0 [u,0,0] | 0,1/2,0 [0,u,0] | 1/2,1/2,0 [u,u,0] |
| 2  | e | 6'mm' | 0,0,z [0,0,0] | 0,0,z [0,0,0] | 0,0,z [0,0,0] |
| 2  | d | 6'm2' | 1/3,2,3,1/2 [0,0,0] | 2/3,1/3,1/2 [0,0,0] | 2/3,1/3,1/2 [0,0,0] |
| 2  | c | 6'm2' | 1/3,2,3,0 [0,0,0] | 2/3,1/3,0 [0,0,0] | 2/3,1/3,0 [0,0,0] |
| 1  | b | 6'mmm' | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |
| 1  | a | 6'mmm' | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |
Symmetry of Special Projections

Along [0,0,1]  \( p6'mm' \)
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,0,0]  \( p2mm1' \)
\[ a^* = c \quad b^* = (a + 2b)/2 \]
Origin at x,0,0

Along [2,1,0]  \( p2'mm' \)
\[ a^* = b/2 \quad b^* = c \]
Origin at x,x/2,0
**Origin** at center (6/mm'\( m' \))

**Asymmetric unit**

\[
\begin{align*}
0 \leq x \leq \frac{2}{3} ; & \quad 0 \leq y \leq \frac{1}{3} ; \quad 0 \leq z \leq \frac{1}{2} ; \quad x \leq \frac{(1+y)}{2} ; \quad y \leq \frac{x}{2} \\
\text{Vertices} & \quad 0,0,0 \quad 1/2,0,0 \quad 2/3,1/3,0 \\
& \quad 0,0,1/2 \quad 1/2,0,1/2 \quad 2/3,1/3,1/2
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1|0,0,0) \\
(2) & \quad 3^* \quad 0,0,z \\
& \quad (3_z|0,0,0) \\
(3) & \quad 3' \quad 0,0,z \\
& \quad (3_z^-|0,0,0) \\
(4) & \quad 2 \quad 0,0,z \\
& \quad (2_z|0,0,0) \\
(5) & \quad 6' \quad 0,0,z \\
& \quad (6_z|0,0,0) \\
(6) & \quad 6' \quad 0,0,z \\
& \quad (6_z^-|0,0,0) \\
(7) & \quad 2' \quad x,x,0 \\
& \quad (2_{xy}|0,0,0)' \\
(8) & \quad 2' \quad x,0,0 \\
& \quad (2_{x}|0,0,0)' \\
(9) & \quad 2' \quad 0,y,0 \\
& \quad (2_{y}|0,0,0)' \\
(10) & \quad 2' \quad x,x,0 \\
& \quad (2_{z}|0,0,0)' \\
(11) & \quad 2' \quad x,2x,0 \\
& \quad (2_{2x}|0,0,0)' \\
(12) & \quad 2' \quad 2x,x,0 \\
& \quad (2_{2x}|0,0,0)'
\end{align*}
\]
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

<table>
<thead>
<tr>
<th>Positions</th>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>24 r 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) ( \bar{x} \cdot \bar{y} \cdot \bar{z} \cdot [\bar{u} \cdot \bar{v} \cdot \bar{w}] )</td>
</tr>
<tr>
<td></td>
<td>(7) ( y \cdot x \cdot z \cdot [v \cdot u \cdot w] )</td>
</tr>
<tr>
<td></td>
<td>(10) ( y \cdot x \cdot z \cdot [v, u \cdot w] )</td>
</tr>
<tr>
<td></td>
<td>(13) ( x \cdot x + y \cdot z \cdot [v, u \cdot w] )</td>
</tr>
<tr>
<td></td>
<td>(16) ( x \cdot y \cdot z \cdot [v, u \cdot w] )</td>
</tr>
<tr>
<td></td>
<td>(19) ( y \cdot x \cdot z \cdot [v, u \cdot w] )</td>
</tr>
<tr>
<td></td>
<td>(22) ( y \cdot x \cdot z \cdot [v, u \cdot w] )</td>
</tr>
</tbody>
</table>

12 q m.. x,y,1/2 [0,0,w] \( \bar{y} \cdot x-y \cdot 1/2 [0,0,w] \) \( x+y \cdot x,1/2 [0,0,w] \)
| | x,y,1/2 [0,0,w] \( y \cdot x+y \cdot 1/2 [0,0,w] \) \( x-y \cdot x,1/2 [0,0,w] \)
| | y,x,1/2 [0,0,w] \( x-y \cdot y,1/2 [0,0,w] \) \( x+y \cdot x,1/2 [0,0,w] \)
| | \( \bar{y} \cdot x \cdot 1/2 [0,0,w] \) \( \bar{x} \cdot x \cdot 1/2 [0,0,w] \) \( \bar{x} \cdot y \cdot 1/2 [0,0,w] \)

12 p m.. x,y,0 [0,0,w] \( \bar{y} \cdot x \cdot y \cdot 0 [0,0,w] \) \( x+y \cdot x,0 [0,0,w] \)
| | \( \bar{x} \cdot y \cdot 0 [0,0,w] \) \( \bar{y} \cdot x \cdot y \cdot 0 [0,0,w] \) \( x-y \cdot x,0 [0,0,w] \)
| | y,x,0 [0,0,w] \( x-y \cdot y \cdot 0 [0,0,w] \) \( \bar{x} \cdot x \cdot y \cdot 0 [0,0,w] \)
| | \( \bar{y} \cdot x \cdot y \cdot 0 [0,0,w] \) \( \bar{x} \cdot x \cdot y \cdot 0 [0,0,w] \) \( x-y \cdot y,0 [0,0,w] \)
| 12 o  | .m'  | $x,2x,z [u,2u,w]$ | $2x,x,z [2u,u,w]$ | $x,x,z [u,u,w]$ |
|       |      | $x,2x,z [u,2u,w]$ | $2x,x,z [2u,u,w]$ | $x,x,z [u,u,w]$ |
|       |      | $2x,x,z [2u,u,w]$ | $x,2x,z [u,2u,w]$ | $x,x,z [u,u,w]$ |
|       |      | $2x,x,z [2u,u,w]$ | $x,2x,z [u,2u,w]$ | $x,x,z [u,u,w]$ |
| 12 n  | .m'  | $x,0,z [u,0,w]$   | $0,x,z [0,u,w]$   | $x,x,z [u,u,w]$ |
|       |      | $x,0,z [u,0,w]$   | $0,x,z [0,u,w]$   | $x,x,z [u,u,w]$ |
|       |      | $0,x,z [0,u,w]$   | $x,0,z [0,u,w]$   | $x,x,z [u,u,w]$ |
|       |      | $0,x,z [0,u,w]$   | $x,0,z [0,u,w]$   | $x,x,z [u,u,w]$ |
| 6 m   | mm'2' | $x,2x,1/2 [0,0,w]$ | $2x,x,1/2 [0,0,w]$ | $x,x,1/2 [0,0,w]$ |
|       |      | $x,2x,1/2 [0,0,w]$ | $2x,x,1/2 [0,0,w]$ | $x,x,1/2 [0,0,w]$ |
| 6 l   | mm'2' | $x,2x,0 [0,0,w]$  | $2x,0,x [0,0,w]$  | $x,x,0 [0,0,w]$  |
|       |      | $x,2x,0 [0,0,w]$  | $2x,0,x [0,0,w]$  | $x,x,0 [0,0,w]$  |
| 6 k   | m2'm' | $x,0,1/2 [0,0,w]$ | $0,x,1/2 [0,0,w]$ | $x,x,1/2 [0,0,w]$ |
|       |      | $x,0,1/2 [0,0,w]$ | $0,x,1/2 [0,0,w]$ | $x,x,1/2 [0,0,w]$ |
| 6 j   | m2'm' | $x,0,0 [0,0,w]$   | $0,x,0 [0,0,w]$   | $x,x,0 [0,0,w]$   |
|       |      | $x,0,0 [0,0,w]$   | $0,x,0 [0,0,w]$   | $x,x,0 [0,0,w]$   |
| 6 i   | 2m'm' | $1/2,0,z [0,0,w]$ | $0,1/2,z [0,0,w]$ | $1/2,1/2,z [0,0,w]$ |
|       |      | $0,1/2,z [0,0,w]$ | $1/2,0,z [0,0,w]$ | $1/2,1/2,z [0,0,w]$ |
| 4 h   | 3m'  | $1/3,2/3,z [0,0,w]$ | $2/3,1/3,z [0,0,w]$ | $1/3,2/3,z [0,0,w]$ |
| 3 g   | mm'm' | $1/2,0,1/2 [0,0,w]$ | $0,1/2,1/2 [0,0,w]$ | $1/2,1/2,1/2 [0,0,w]$ |
| 3 f   | mm'm' | $1/2,0,0 [0,0,w]$  | $0,1/2,0 [0,0,w]$  | $1/2,1/2,0 [0,0,w]$ |
| 2 e   | 6m'm' | $0,0,z [0,0,w]$   | $0,0,z [0,0,w]$   | $0,0,z [0,0,w]$   |
| 2 d   | 6m'2' | $3/2,3,1/2 [0,0,w]$ | $2/3,1/3,1/2 [0,0,w]$ | $3/2,3,1/2 [0,0,w]$ |
| 2 c   | 6m'2' | $3/2,3,0 [0,0,w]$  | $2/3,1/3,0 [0,0,w]$ | $3/2,3,0 [0,0,w]$  |
| 1 b   | 6/mm'm' | $0,0,1/2 [0,0,w]$ | $0,0,1/2 [0,0,w]$ | $0,0,1/2 [0,0,w]$ |
| 1 a   | 6/mm'm' | $0,0,0 [0,0,w]$ | $0,0,0 [0,0,w]$ | $0,0,0 [0,0,w]$ |
Symmetry of Special Projections

Along [0,0,1] p6mm1'
\[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along [1,0,0] p2'mm'
\[ \mathbf{a}^* = \mathbf{c}, \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \]
Origin at x,0,0

Along [2,1,0] p2'mm'
\[ \mathbf{a}^* = \mathbf{c}, \quad \mathbf{b}^* = \mathbf{b}/2 \]
Origin at x,x/2,0
**Origin** at center (6/m'm'm')

**Asymmetric unit**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 2/3</td>
<td>0 ≤ y ≤ 1/3</td>
<td>0 ≤ z ≤ 1/2</td>
</tr>
<tr>
<td>x ≤ (1+y)/2</td>
<td>y ≤ x/2</td>
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</tr>
</tbody>
</table>

**Vertices**

<p>| | | |</p>
<table>
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<tr>
<th></th>
<th></th>
<th></th>
</tr>
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<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
</tr>
<tr>
<td>0,0,1/2</td>
<td>1/2,0,1/2</td>
<td>2/3,1/3,1/2</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

(1) 1
(1 | 0,0,0)

(2) 3^* 0,0,z
(3 | z | 0,0,0)

(3) 3^-1 0,0,z
(3 | z^-1 | 0,0,0)

(4) 2 0,0,z
(2 | z | 0,0,0)

(5) 6^-1 0,0,z
(6 | z^-1 | 0,0,0)

(6) 6^* 0,0,z
(6 | 0,0,0)

(7) 2 x,x,0
(2 | x | 0,0,0)

(8) 2 x,0,0
(2 | z | 0,0,0)

(9) 2 0,y,0
(2 | y | 0,0,0)

(10) 2 x,x,0
(2 | x | 0,0,0)

(11) 2 x,2x,0
(2 | 2z | 0,0,0)

(12) 2 2x,x,0
(2 | 2z | 0,0,0)
Continued

(13) $\overline{1}$' 0,0,0 
(14) $\overline{3}$' 0,0,0; 0,0,0 
(15) $\overline{3}$' 0,0,0; 0,0,0 

(16) m' x,y,0 
(m$_{x}$|0,0,0)'
(17) $6'$ 0,0,0; 0,0,0 
(6$_{z}$|0,0,0)'
(18) $6'$ 0,0,0; 0,0,0 
(6$_{z}$|0,0,0)'

(19) m' x,x,z 
(m$_{y}$|0,0,0)'
(20) m' x,2x,z 
(m$_{y}$|0,0,0)'
(21) m' 2x,x,z 
(m$_{y}$|0,0,0)'

Generators selected 
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

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</tbody>
</table>

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<tr>
<th>24</th>
<th>r</th>
<th>1</th>
<th>x,y,z [u,v,w]</th>
<th>(1) x,y,z [u,v,w]</th>
<th>(2) y,x-y,z [v-u-v,w]</th>
<th>(3) $x+y,x,z [u+v,u,w]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4)</td>
<td>x,y,z [u,v,w]</td>
<td>(5) y,x+y,z [v-u+v,w]</td>
<td>(6) x-y,x,z [u-v,u,w]</td>
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</tr>
<tr>
<td>(7)</td>
<td>y,x,z [v,u,w]</td>
<td>(8) x-y,z [u-v,v,w]</td>
<td>(9) x,x-y,z [u,u+v,w]</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>(10)</td>
<td>y,x,z [v,u,w]</td>
<td>(11) x+y,z [u+v,v,w]</td>
<td>(12) x,x-y,z [u-u+v,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(13)</td>
<td>x,y,z [v,u,w]</td>
<td>(14) y,x-y,z [v-u+v,w]</td>
<td>(15) x-y,x-z [u-v,u,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(16)</td>
<td>x,y,z [v,u,w]</td>
<td>(17) x+y,z [v-u+v,w]</td>
<td>(18) x+y,x,z [u+v,u,w]</td>
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</tr>
<tr>
<td>(19)</td>
<td>y,x,z [v,u,w]</td>
<td>(20) x+y,y,z [u+v,v,w]</td>
<td>(21) x,x-y,z [u-u+v,w]</td>
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<tr>
<td>(22)</td>
<td>y,x,z [v,u,w]</td>
<td>(23) x-y,x,z [u-u+v,w]</td>
<td>(24) x,x+y,z [u-u+v,w]</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>12</th>
<th>q</th>
<th>m':</th>
<th>x,y,1/2 [u,v,0]</th>
<th>x,y,1/2 [u,v,0]</th>
<th>x+y,x,1/2 [u+v,u,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,y,1/2 [u,v,0]</td>
<td>y,x-y,1/2 [v-u-v,0]</td>
<td>x-y,x,1/2 [u-v,u,0]</td>
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<tr>
<td>y,x,1/2 [v,u,0]</td>
<td>y,x+y,1/2 [v-u+v,0]</td>
<td>x+y,x,1/2 [u+v,u,0]</td>
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<tr>
<td>y,x,1/2 [v,u,0]</td>
<td>x-y,z,1/2 [u-u+v,0]</td>
<td>x,x-y,1/2 [u-u+v,0]</td>
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<th>x,y,0 [u,v,0]</th>
<th>x+y,x,0 [u+v,u,0]</th>
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<td>x+y,x,0 [u+v,u,0]</td>
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<tr>
<td>x,y,0 [u,v,0]</td>
<td>y,x+y,0 [v,u+v,0]</td>
<td>x-x,y,0 [u-u+v,0]</td>
<td></td>
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<tr>
<td>x,y,0 [v,u,0]</td>
<td>x-y,z,0 [u-u+v,0]</td>
<td>x-x,y,0 [u-u+v,0]</td>
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<td></td>
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<tr>
<td>y,x,0 [v,u,0]</td>
<td>x-y,y,0 [u-u+v,0]</td>
<td>x-x,y,0 [u-u+v,0]</td>
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</tr>
<tr>
<td>12 o</td>
<td>.m'</td>
<td>x,2x,z [u,2u,w]</td>
<td>2x,x,z [2u,2u,w]</td>
<td>x,x,z [u,u,w]</td>
<td></td>
</tr>
<tr>
<td>12 n</td>
<td>.m'</td>
<td>x,0,z [u,0,w]</td>
<td>0,x,z [0,u,w]</td>
<td>x,x,z [u,u,w]</td>
<td></td>
</tr>
<tr>
<td>6 m</td>
<td>m'2m'</td>
<td>x,2x,1/2 [u,2u,0]</td>
<td>2x,x,1/2 [2u,2u,0]</td>
<td>x,x,1/2 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>6 l</td>
<td>m'2m'</td>
<td>x,2x,0 [u,2u,0]</td>
<td>2x,x,0 [2u,2u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>6 k</td>
<td>m'2m'</td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,x,1/2 [0,u,0]</td>
<td>x,x,1/2 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>6 j</td>
<td>m'2m'</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
<td>x,x,0 [u,u,0]</td>
<td></td>
</tr>
<tr>
<td>6 i</td>
<td>m'2m'</td>
<td>1/2,0,z [0,0,w]</td>
<td>0,1/2,z [0,0,w]</td>
<td>1/2,1/2,z [0,0,w]</td>
<td></td>
</tr>
<tr>
<td>4 h</td>
<td>3m'</td>
<td>1/3,2/3,z [0,0,w]</td>
<td>2/3,1/3,z [0,0,w]</td>
<td>1/3,2/3,z [0,0,w]</td>
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</tr>
<tr>
<td>3 g</td>
<td>m'm'm'</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>3 f</td>
<td>m'm'm'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 e</td>
<td>6m'm'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<tr>
<td>2 d</td>
<td>6m'2</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
<td>2/3,1/3,1/2 [0,0,0]</td>
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<tr>
<td>2 c</td>
<td>6m'2</td>
<td>1/3,2/3,0 [0,0,0]</td>
<td>2/3,1/3,0 [0,0,0]</td>
<td></td>
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</tr>
<tr>
<td>1 b</td>
<td>6m'm'm'</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 a</td>
<td>6m'm'm'</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along $[0,0,1]$ p6m'm'
\[ \mathbf{a}^* = \mathbf{a}, \quad \mathbf{b}^* = \mathbf{b} \]
Origin at 0,0,z

Along $[1,0,0]$ p2m'm'
\[ \mathbf{a}^* = \mathbf{c}, \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \]
Origin at x,0,0

Along $[2,1,0]$ p2m'm'
\[ \mathbf{a}^* = \mathbf{c}, \quad \mathbf{b}^* = \mathbf{b}/2 \]
Origin at x,x/2,0
Origin at center (6/mmm)

Asymmetric unit

\[
0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{3}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq \frac{1+y}{2}; \quad y \leq \frac{x}{2}
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* 0,0,z \\
(3) & \quad 3^- 0,0,z \\
(4) & \quad 2 0,0,z \\
(5) & \quad 6^- 0,0,z \\
(6) & \quad 6^- 0,0,z \\
(7) & \quad 2 x,x,0 \\
(8) & \quad 2 x,0,0 \\
(9) & \quad 2 0,y,0 \\
(10) & \quad 2 x,x,0 \\
(11) & \quad 2 x,2x,0 \\
(12) & \quad 2 2x,x,0
\end{align*}
\]
Continued

(13) $\bar{1}$ 0,0,0
(14) $\bar{3}^+$ 0,0,z; 0,0,0
(15) $\bar{3}^-$ 0,0,z; 0,0,0

(16) $m$ x,y,0
$\langle m \rangle$ 0,0,0
(17) $\bar{6}^-$ 0,0,z; 0,0,0
$\langle \bar{6} \rangle$ 0,0,0
(18) $\bar{6}^+$ 0,0,z; 0,0,0
$\langle \bar{6} \rangle$ 0,0,0

(19) $m$ x,x,z
$\langle m \rangle$ 0,0,0
(20) $m$ x,2x,z
$\langle m \rangle$ 0,0,0
(21) $2x$,x,z
$\langle m \rangle$ 0,0,0

(22) $m$ x,x,z
$\langle m \rangle$ 0,0,0
(23) $m$ x,0,z
$\langle m \rangle$ 0,0,0
(24) m 0,y,z
$\langle m \rangle$ 0,0,0

For (0,0,1)'+ set

(1) $t'(0,0,1)$
(2) $3^+ (0,0,1) 0,0,z$
(3) $3^- (0,0,1) 0,0,z$
(4) $2' (0,0,1) 0,0,z$
(5) $6^- (0,0,1) 0,0,z$
(6) $6^+ (0,0,1) 0,0,z$
(7) $2' (x,x,1/2)$
(8) $2' (x,0,1/2)$
(9) $2' (0,y,1/2)$
(10) $2' (x,x,1/2)$
(11) $2' (x,2x,1/2)$
(12) $2' (x,2x,1/2)$
(13) $\bar{1}^+ (0,0,1/2)$
(14) $\bar{3}^+ (0,0,1) 0,0,1/2$
(15) $\bar{3}^- (0,0,1) 0,0,1/2$
(16) $m' (x,y,1/2)$
(17) $\bar{6}^+ (x,y,1/2)$
(18) $\bar{6}^- (x,y,1/2)$
(19) $c' (0,0,1) x,x,z$
(20) $c' (0,0,1) x,2x,z$
(21) $c' (0,0,1) 2x,x,z$
(22) $c' (0,0,1) x,x,z$
(23) $c' (0,0,1) x,0,z$
(24) $c' (0,0,1) 0,y,z$

Generators selected
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7); (13).

Positions

<table>
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<th>Coordinates</th>
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Continued

\[ (13) \bar{x}, \bar{y}, \bar{z} \] \[ v, u, w \]

\[ (14) y, x+y, \bar{z} \] \[ v, u-v, w \]

\[ (15) x-y, x, \bar{z} \] \[ u+v, u, w \]

\[ (16) x, y, z \] \[ u, v, w \]

\[ (17) \bar{y}, x-y, z \] \[ v, u+v, w \]

\[ (18) \bar{x}+y, x, \bar{z} \] \[ u-v, u, w \]

\[ (19) \bar{y}, x, z \] \[ v, u, w \]

\[ (20) \bar{x}+y, y, z \] \[ u-v, v, w \]

\[ (21) \bar{x}, x-y, z \] \[ u, u+v, w \]

\[ (22) x, y, z \] \[ v, u, w \]

\[ (23) x, y, z \] \[ u+v, v, w \]

\[ (24) x, x+y, z \] \[ u, u+v, w \]

\[ 24 q m'.. \]

\[ x, y, 1/2 \] \[ u, v, 0 \]

\[ \bar{x}, y, 1/2 \] \[ v, u, 0 \]

\[ y, x, 1/2 \] \[ v, u, 0 \]

\[ \bar{y}, \bar{x}, 1/2 \] \[ v, u, 0 \]

\[ x, y, 0 \] \[ 0, 0, w \]

\[ \bar{x}, y, 0 \] \[ 0, 0, w \]

\[ y, x, 0 \] \[ 0, 0, w \]

\[ \bar{y}, x, 0 \] \[ 0, 0, w \]

\[ 24 p m.. \]

\[ x, 2x, z \] \[ u, 0, 0 \]

\[ \bar{x}, 2x, z \] \[ u, 0, 0 \]

\[ 2x, x, \bar{z} \] \[ 0, u, 0 \]

\[ 2x, x, z \] \[ u, 0, 0 \]

\[ 0, x, 0 \] \[ 0, 2u, 0 \]

\[ \bar{0}, x, 0 \] \[ 0, 2u, 0 \]

\[ 0, x, \bar{z} \] \[ 2u, 0, 0 \]

\[ \bar{0}, x, \bar{z} \] \[ 2u, 0, 0 \]

\[ 0, 0, \bar{z} \] \[ 2u, 0, 0 \]

\[ \bar{0}, 0, \bar{z} \] \[ 2u, 0, 0 \]

\[ 12 m m'm' \]

\[ x, 2x, 1/2 \] \[ u, 0, 0 \]

\[ \bar{x}, 2x, 1/2 \] \[ u, 0, 0 \]

\[ 2x, x, 0 \] \[ 0, 0, 0 \]

\[ \bar{2}x, x, 0 \] \[ 0, 0, 0 \]

\[ 0, x, 0 \] \[ 0, 0, 0 \]

\[ \bar{0}, x, 0 \] \[ 0, 0, 0 \]

\[ 12 l m'm' \]

\[ x, 0, 1/2 \] \[ 2u, 0, 0 \]

\[ \bar{x}, 0, 1/2 \] \[ 2u, 0, 0 \]

\[ 0, x, 0 \] \[ 0, 0, 0 \]

\[ \bar{0}, x, 0 \] \[ 0, 0, 0 \]

\[ 12 k m'm' \]

\[ x, 0, 0 \] \[ 0, 0, 0 \]

\[ \bar{x}, 0, 0 \] \[ 0, 0, 0 \]

\[ 0, x, 0 \] \[ 0, 0, 0 \]

\[ \bar{0}, x, 0 \] \[ 0, 0, 0 \]

\[ 12 j m'm' \]

\[ x, 0, 0 \] \[ 0, 0, 0 \]

\[ \bar{x}, 0, 0 \] \[ 0, 0, 0 \]

\[ 0, x, 0 \] \[ 0, 0, 0 \]

\[ \bar{0}, x, 0 \] \[ 0, 0, 0 \]
### Symmetry of Special Projections

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<tr>
<td>6</td>
<td>g</td>
<td>m'mm</td>
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<td>mmm</td>
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<td>4</td>
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<td>2</td>
<td>a</td>
<td>6/mmm</td>
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</table>

\[
\begin{align*}
\mathbf{a}^* &= \mathbf{a} \\
\mathbf{b}^* &= \mathbf{b} \\
\mathbf{c}^* &= \mathbf{c} \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 \\
\mathbf{a}^* &= \mathbf{c} \quad \mathbf{b}^* = \mathbf{b}/2
\end{align*}
\]

Origin at 0,0,z  \quad \text{Origin at } x,0,0  \quad \text{Origin at } x,x/2,0
**Origin** at center (6'/mm'm)

**Asymmetric unit**

\[
\begin{align*}
0 & \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1/2; \quad x \leq (1+y)/2; \quad y \leq x/2
\end{align*}
\]

**Vertices**

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 \\
0,0,1/2 & \quad 1/2,0,1/2 & \quad 2/3,1/3,1/2
\end{align*}
\]

**Symmetry Operations**

For \((0,0,0) + \text{set} \)

\[
\begin{align*}
(1) \quad & 1 \\
(1') & 0,0,0 \\
(10) & 2' \quad x,x,0 & (2) & 3' \quad 0,0,z & (3) & 3' \quad 0,0,z \\
& (1|0,0,0) & (3|_z,0,0,0) & (3|_z,0,0,0) & (3|_z,0,0,0) \\
(4) & 2' \quad 0,0,z & (5) & 6' \quad 0,0,z & (6) & 6' \quad 0,0,z \\
& (2|_z,0,0,0) & (6|_z,0,0,0) & (6|_z,0,0,0) & (6|_z,0,0,0) \\
(7) & 2 \quad x,x,0 & (8) & 2 \quad x,0,0 & (9) & 2 \quad 0,y,0 \\
& (2|_{xy},0,0,0) & (2|_x,0,0,0) & (2|_y,0,0,0) & (2|_y,0,0,0) \\
(10) & 2' \quad x,x,0 & (11) & 2' \quad 2x,0,0 & (12) & 2' \quad 0,x,x,0 \\
& (2|_z,0,0,0) & (2|_2,0,0,0') & (2|_z,0,0,0) & (2|_z,0,0,0)'
\end{align*}
\]
Continued

| 13 | $t'$ 0,0,0 |
| 14 | $3^{+}$ 0,0,z; 0,0,0 |
| 15 | $3^{-}$ 0,0,z; 0,0,0 |

| 16 | m x,y,0 |
| 17 | $6^{-}$ 0,0,z; 0,0,0 |
| 18 | $6^{+}$ 0,0,z; 0,0,0 |

| 19 | m' x,z |
| 20 | m' x,2x,z |
| 21 | m' 2x,z |

| 22 | m x,z |
| 23 | m x,0,z |
| 24 | m 0,y,z |

For (0,0,1)'+ set

| 1 | $t'$ (0,0,1) |
| 2 | $3^{+}$ (0,0,1) 0,0,z |
| 3 | $3^{-}$ (0,0,1) 0,0,z |

| 4 | 2 (0,0,1) 0,0,z |
| 5 | $6^{-}$ (0,0,1) 0,0,z |
| 6 | $6^{+}$ (0,0,1) 0,0,z |

| 7 | 2' x,x,1/2 |
| 8 | 2' x,0,1/2 |
| 9 | 2' 0,y,1/2 |

| 10 | 2 x,x,1/2 |
| 11 | 2 x,2x,1/2 |
| 12 | 2 2x,1/2 |

| 13 | $t$ 0,0,1/2 |
| 14 | $3^{+}$ 0,0,z; 0,0,1/2 |
| 15 | $3^{-}$ 0,0,z; 0,0,1/2 |

| 16 | m' x,y,1/2 |
| 17 | $6^{-}$ 0,0,z; 0,0,1/2 |
| 18 | $6^{+}$ 0,0,z; 0,0,1/2 |

| 19 | c (0,0,1) x,z |
| 20 | c (0,0,1) x,2x,z |
| 21 | c (0,0,1) 2x,z |

| 22 | c' (0,0,1) x,z |
| 23 | c' (0,0,1) x,0,z |
| 24 | c' (0,0,1) 0,y,z |

Generators selected

(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7); (13).

Positions

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<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
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<td>(3) $\bar{x}$+y,x,z [u+v,u,w]</td>
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**Symmetry of Special Projections**

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<th>Along [1,0,0] p2mm</th>
<th>Along [2,1,0] p2mm1'</th>
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<td>( \mathbf{a}^* = \mathbf{c} ) ( \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 )</td>
<td>( \mathbf{a}^* = \mathbf{c} ) ( \mathbf{b}^* = \mathbf{b}/2 )</td>
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<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin at center (6'/mmm')

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/3; \quad 0 \leq z \leq 1/2; \quad x < (1+y)/2; \quad y < x/2 \]

Vertices

\[
\begin{array}{ccc}
0,0,0 & 1/2,0,0 & 2/3,1/3,0 \\
0,0,1/2 & 1/2,0,1/2 & 2/3,1/3,1/2
\end{array}
\]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \ 0,0,z \\
(3) & \quad 3' \ 0,0,z \\
(4) & \quad 2' \ 0,0,z \\
(5) & \quad 6' \ 0,0,z \\
(6) & \quad 6'' \ 0,0,z \\
(7) & \quad 2' \ x,x,0 \\
(8) & \quad 2' \ x,0,0 \\
(9) & \quad 2' \ 0,y,0 \\
(10) & \quad 2 \ x,x,0 \\
(11) & \quad 2 \ x,2x,0 \\
(12) & \quad 2 \ 2x,x,0
\end{align*}
\]
Continued

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>(0,0,0) + (0,0,1)' +</td>
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<td>(1) x,y,z [u,v,w]</td>
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<td>(2) y,x-y,z [v,-u-v,w]</td>
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<td>(3) x+y,x,z [u+v,u+w]</td>
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<td>(7) y,x,z [v,-u,w]</td>
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<td>(8) x-y,y,z [u+v,v+w]</td>
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<td></td>
<td>(10) y,x,z [v,u,w]</td>
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<tr>
<td></td>
<td></td>
<td>(11) x+y,y,z [u+v,v+w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(12) x,x-y,z [u,u-v,w]</td>
</tr>
</tbody>
</table>

191.12.1474 - 2 - 3231
(13) $x, y, z \ [u, v, w]$

(14) $y, x + y, z \ [v, u + v, w]$

(15) $x - y, x, z \ [u, v, u + w]$

(16) $x, y, z \ [u, v, w]$

(17) $y, x - y, z \ [v, u + v, w]$

(18) $x + y, x, z \ [u - v, u, w]$

(19) $y, x, z \ [v, u, w]$

(20) $x + y, y, z \ [u - v, v, w]$

(21) $x, x - y, z \ [u, u + v, w]$

$24 \ q \ \text{m}'..$

$x, y, 1/2 \ [u, v, 0]$

$y, x, 1/2 \ [v, u, 0]$

$x, y, 1/2 \ [u, v, 0]$

$y, x, 1/2 \ [v, u, 0]$

$y, x, 1/2 \ [v, u, 0]$

$x + y, 1/2 \ [u, v, 0]$

$x + y, 1/2 \ [u, v, 0]$

$x + y, 1/2 \ [u, v, 0]$

$x + y, 1/2 \ [u, v, 0]$

$x + y, 1/2 \ [u, v, 0]$

$x + y, 1/2 \ [u, v, 0]$

$24 \ p \ \text{m}..$

$x, y, 0 \ [0, 0, w]$

$y, x, 0 \ [0, 0, w]$

$x, y, 0 \ [0, 0, w]$

$y, x, 0 \ [0, 0, w]$

$y, x, 0 \ [0, 0, w]$

$y + x, 0 \ [0, 0, w]$

$y + x, 0 \ [0, 0, w]$

$y + x, 0 \ [0, 0, w]$

$y + x, 0 \ [0, 0, w]$

$24 \ o \ \text{m}..$

$x, 2x, z \ [u, 0, 0]$

$2x, x, z \ [0, u, 0]$

$x, 2x, z \ [u, 0, 0]$

$2x, x, z \ [0, u, 0]$

$x, 2x, z \ [u, 0, 0]$

$2x, x, z \ [0, u, 0]$

$2x, x, z \ [0, u, 0]$

$2x, x, z \ [0, u, 0]$

$2x, x, z \ [0, u, 0]$

$0, x, z \ [0, 0, w]$

$0, x, z \ [0, 0, w]$

$0, x, z \ [0, 0, w]$

$0, x, z \ [0, 0, w]$

$0, x, z \ [0, 0, w]$

$12 \ m \ \text{mm}2$

$x, 2x, 1/2 \ [u, 0, 0]$

$x, 2x, 1/2 \ [u, 0, 0]$

$x, 2x, 1/2 \ [u, 0, 0]$

$x, 2x, 1/2 \ [u, 0, 0]$

$x, 2x, 1/2 \ [u, 0, 0]$

$x, 2x, 1/2 \ [u, 0, 0]$

$12 \ l \ \text{mm}2$

$x, 2x, 0 \ [0, 0, 0]$

$x, 2x, 0 \ [0, 0, 0]$

$x, 2x, 0 \ [0, 0, 0]$

$x, 2x, 0 \ [0, 0, 0]$

$x, 2x, 0 \ [0, 0, 0]$

$x, 2x, 0 \ [0, 0, 0]$

$12 \ k \ \text{m}'2\text{m}'$

$x, 0, 1/2 \ [u, 0, 0]$

$x, 0, 1/2 \ [u, 0, 0]$

$x, 0, 1/2 \ [u, 0, 0]$

$x, 0, 1/2 \ [u, 0, 0]$

$x, 0, 1/2 \ [u, 0, 0]$

$x, 0, 1/2 \ [u, 0, 0]$

$12 \ j \ \text{m}2\text{m}'$

$x, 0, 0 \ [0, 0, w]$

$x, 0, 0 \ [0, 0, w]$

$x, 0, 0 \ [0, 0, w]$

$x, 0, 0 \ [0, 0, w]$

$x, 0, 0 \ [0, 0, w]$

$x, 0, 0 \ [0, 0, w]$
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<tr>
<th>12</th>
<th>i</th>
<th>2'mm'</th>
<th>1/2,0,z [u,0,0]</th>
<th>0,1/2,z [0,u,0]</th>
<th>1/2,1/2,z [u,u,0]</th>
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<td>0,1/2,z [0,u,0]</td>
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<tr>
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<td>m'mm'</td>
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<td>0,1/2,1/2 [0,u,0]</td>
<td>1/2,1/2,1/2 [u,u,0]</td>
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<tr>
<td>6</td>
<td>f</td>
<td>mmm'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<tr>
<td>4</td>
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<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2</td>
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<td>6'/m'mm'</td>
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</tr>
<tr>
<td>2</td>
<td>a</td>
<td>6'/mmm'</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
\[a^* = a \quad b^* = b\]  
Origin at 0,0,z

Along [1,0,0] p2mm1'  
\[a^* = c \quad b^* = (a + 2b)/2\]  
Origin at x,0,0

Along [2,1,0] p2x, 2mm  
\[a^* = c \quad b^* = b/2\]  
Origin at x,x/2,0
**Origin** at center (6/mm'm')

**Asymmetric unit**
- \(0 \leq x \leq 2/3;\) \(0 \leq y \leq 1/3;\) \(0 \leq z \leq 1/2;\) \(x \leq (1+y)/2;\) \(y \leq x/2\)
- Vertices: \((0,0,0), (1/2,0,0), (2/3,1/3,0), (0,0,1/2), (1/2,0,1/2), (2/3,1/3,1/2)\)

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \((1)\) 1
   - \((1|0,0,0)\)

2. \((2)\) 3* 0,0,z
   - \((3_z|0,0,0)\)
   - \((3_z^-1|0,0,0)\)

3. \((3)\) 3* 0,0,z
   - \((3_z|0,0,0)\)
   - \((3_z^-1|0,0,0)\)

4. \((4)\) 2 0,0,z
   - \((2_z|0,0,0)\)
   - \((6^-1|0,0,0)\)
   - \((6|0,0,0)\)

5. \((5)\) 6* 0,0,z
   - \((6_z|0,0,0)\)

6. \((6)\) 6* 0,0,z
   - \((6|0,0,0)\)

7. \((7)\) 2' x,x,0
   - \((2_{xy}|0,0,0)'\)
   - \((2_{xy}|0,0,0)'\)

8. \((8)\) 2' x,0,0
   - \((2_{z}|0,0,0)'\)

9. \((9)\) 2' 0,y,0
   - \((2_{y}|0,0,0)'\)

10. \((10)\) 2' x,x,0
    - \((2_z|0,0,0)'\)

11. \((11)\) 2' 2x,0
    - \((2_{z}|0,0,0)'\)

12. \((12)\) 2' 2x,0
    - \((2_{z}|0,0,0)'\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t'(0,0,1); (2); (4); (7); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<tbody>
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<td>48</td>
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Coordinates

(0,0,0) + (0,0,1)' +

<table>
<thead>
<tr>
<th>1</th>
<th>x,y,z [u,v,w]</th>
<th>2</th>
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<th>3</th>
<th>$\bar{x}$+y,$\bar{x}$,z [u+v,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
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<td>$\bar{x}$,y,z [u,-v,w]</td>
<td>5</td>
<td>y,$\bar{x}$+z [v,u+v,w]</td>
<td>6</td>
<td>x-y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td>7</td>
<td>y,x,z [v,u,w]</td>
<td>8</td>
<td>x-y,$\bar{y}$,z [u+v,v,w]</td>
<td>9</td>
<td>$\bar{x}$,x+y,z [u,u-v,w]</td>
</tr>
<tr>
<td>10</td>
<td>$\bar{y}$,x,z [v,u,w]</td>
<td>11</td>
<td>$\bar{x}$+y,y,z [u-v,v,w]</td>
<td>12</td>
<td>x,x-y,z [u,u-v+w]</td>
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<td>Continued</td>
<td>191.13.1475</td>
<td>P&lt;sub&gt;2&lt;/sub&gt; 6/mm'm'</td>
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<tr>
<td>(13) (x, y, z [u, v, w])</td>
<td>(14) (y, x + y, z [v, u-v, w])</td>
<td>(15) (x-y, x, z [u+v, u, w])</td>
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<tr>
<td>(16) (x, y, z [u, v, w])</td>
<td>(17) (y, x-y, z [v, u+v, w])</td>
<td>(18) (x+y, x, z [u-v, u, w])</td>
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<tr>
<td>(19) (y, x, z [v, u, w])</td>
<td>(20) (x+y, y, z [u+v, v, w])</td>
<td>(21) (x, x-y, z [u-u+v, v, w])</td>
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<td>(22) (y, x, z [v, u, w])</td>
<td>(23) (x-y, y, z [u-v, v, w])</td>
<td>(24) (x, x+y, z [u-u=v, v, w])</td>
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<td>(24 \ q \ m')</td>
<td>(x, y, 1/2 [u, v, 0])</td>
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<td></td>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>g</td>
<td>m’mm’</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>f</td>
<td>mm’mm’</td>
<td>1/2,0,0 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,1/2,0 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>e</td>
<td>6m’mm’</td>
<td>0,0,z [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,z [0,0,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>d</td>
<td>6’m’2</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>6’m’2’</td>
<td>1/3,2/3,0 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,0 [0,0,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>b</td>
<td>6/m’mm’</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>6/mm’mm’</td>
<td>0,0,0 [0,0,w]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] 6mm1’

* a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p6m’mm’

* a* = c  b* = (a + 2b)/2
Origin at x,0,1/2

Along [2,1,0] P2a’ 2m’mm’

* a* = c  b* = b/2
Origin at x,x/2,1/2

**Symmetry of Special Projections**

Along [0,0,1] 6mm1’

* a* = a  b* = b
Origin at 0,0,z

Along [1,0,0] p6m’mm’

* a* = c  b* = (a + 2b)/2
Origin at x,0,1/2

Along [2,1,0] P2a’ 2m’mm’

* a* = c  b* = b/2
Origin at x,x/2,1/2
**Origin** at center (6/m) at 6/mcc

**Asymmetric unit**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 2/3;</td>
<td>0 ≤ y ≤ 1/2;</td>
<td>0 ≤ z ≤ 1/4;</td>
</tr>
<tr>
<td>x ≤ (1+y)/2;</td>
<td>y ≤ min (1-x,x)</td>
<td></td>
</tr>
</tbody>
</table>

**Vertices**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
</tr>
<tr>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
<td>2/3,1/3,1/4</td>
</tr>
<tr>
<td>1/2,1/2,0</td>
<td>1/2,1/2,1/4</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. 1
2. 0,0,z
3. 0,0,z
4. 0,0,z
5. 0,0,z
6. 0,0,z
7. 0,0,z
8. 0,0,z
9. 0,0,z
10. 0,0,z
11. 0,0,z
12. 0,0,z

192.1.1476 - 1 - 3238
Continued

192.1.1476

P6/mcc

(13) 1 0,0,0
    (1) 0,0,0
(14) \overline{3'} 0,0,z; 0,0,0
    (3') 0,0,0
(15) \overline{3'} 0,0,z; 0,0,0
    (3'\overline{1}) 0,0,0

(16) m x,y,0
    (m) 0,0,1/2
(17) \overline{6'} 0,0,z; 0,0,0
    (\overline{6'}) 0,0,1/2
(18) \overline{6'} 0,0,z; 0,0,0
    (\overline{6}\overline{1}) 0,0,1/2

(19) c (0,0,1/2) x,x,z
    (m) 0,0,1/2
(20) c (0,0,1/2) x,2x,z
    (m) 0,0,1/2
(21) c (0,0,1/2) 0,y,z
    (m) 0,0,1/2

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

24 m 1
(1) x,y,z [u,v,w]
    (2) y,x-y,z [v,-u,-w]
    (3) x+y,x,z [u+v,u,w]
(4) x,y,z [u,v,w]
    (5) y,x+y,z [v,u+v,w]
    (6) x,y,z [u-v,u,w]
(7) y,x,z+1/2 [v,u,w]
    (8) x-y,y,z+1/2 [u-v,-w]
    (9) x,x+y,z+1/2 [u,u+v,w]
(10) y,x,z+1/2 [v,u,w]
    (11) x+y,y,z+1/2 [u+v,v,w]
    (12) x,x+y,z+1/2 [u-u,v,w]
(13) x,y,z [u,v,w]
    (14) y,x+y,z [v,-u,-w]
    (15) x+y,x,z [u+v,u,w]
(16) x,y,z [u,v,w]
    (17) y,x+y,z [v,u+v,w]
    (18) x+y,x,z [u-u,v,w]
(19) y,x,z+1/2 [v,u,w]
    (20) x+y,y,z+1/2 [u-v,-w]
    (21) x,x+y,z+1/2 [u,u+v,w]
(22) y,x,z+1/2 [v,-u,-w]
    (23) x-y,y,z+1/2 [u,-v,v]
    (24) x,x+y,z+1/2 [u-u,v,w]

12 l m...
    x,y,0 [0,0,w]
    y,x,0 [0,0,w]
    x+y,x,0 [0,0,w]
    y,x,1/2 [0,0,w]
    y,x,1/2 [0,0,w]
    x-y,y,1/2 [0,0,w]
    x,y,1/2 [0,0,w]
    x,y,1/2 [0,0,w]
    x+y,y,1/2 [0,0,w]
    x,x-y,1/2 [0,0,w]

12 k ..2
    x,2x,1/4 [u,2u,0]
    2x,x,1/4 [2u,0]
    x,x,1/4 [u,0]
    x,2x,1/4 [u,2u,0]
    2x,x,1/4 [2u,0]
    x,x,1/4 [u,0]
    x,2x,3/4 [u,2u,0]
    2x,x,3/4 [2u,0]
    x,x,3/4 [u,0]
    x,2x,3/4 [u,2u,0]
    2x,x,3/4 [2u,0]
    x,x,3/4 [u,0]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 j 2</td>
<td>$x,0,1/4 [u,0,0]$</td>
<td>$0,x,1/4 [0,u,0]$</td>
</tr>
<tr>
<td></td>
<td>$\bar{x},0,1/4 [\bar{u},0,0]$</td>
<td>$0,\bar{x},1/4 [0,\bar{u},0]$</td>
</tr>
<tr>
<td></td>
<td>$\bar{x},0,3/4 [u,0,0]$</td>
<td>$0,\bar{x},3/4 [0,u,0]$</td>
</tr>
<tr>
<td></td>
<td>$x,0,3/4 [u,0,0]$</td>
<td>$0,x,3/4 [0,u,0]$</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i 2</td>
<td>$1/2,0,z [0,0,w]$</td>
<td>$0,1/2,z [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$0,1/2,z+1/2 [0,0,w]$</td>
<td>$1/2,0,z+1/2 [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$1/2,0,z [0,0,w]$</td>
<td>$0,1/2,z [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$0,1/2,z+1/2 [0,0,w]$</td>
<td>$1/2,0,z+1/2 [0,0,w]$</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 h 3</td>
<td>$1/3,2/3,z [0,0,w]$</td>
<td>$2/3,1/3,z [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$2/3,1/3,z [0,0,w]$</td>
<td>$1/3,2/3,z [0,0,w]$</td>
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</tbody>
</table>

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<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 g 2m</td>
<td>$1/2,0,0 [0,0,w]$</td>
<td>$0,1/2,0 [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$0,1/2,1/2 [0,0,w]$</td>
<td>$1/2,0,1/2 [0,0,w]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 f 222</td>
<td>$1/2,0,1/4 [0,0,0]$</td>
<td>$0,1/2,1/4 [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td>$1/2,0,3/4 [0,0,0]$</td>
<td>$0,1/2,3/4 [0,0,0]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 e 6</td>
<td>$0,0,z [0,0,w]$</td>
<td>$0,0,z+1/2 [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$0,0,z+1/2 [0,0,w]$</td>
<td>$0,0,z [0,0,w]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 d 6</td>
<td>$1/3,2/3,0 [0,0,w]$</td>
<td>$2/3,1/3,0 [0,0,w]$</td>
</tr>
<tr>
<td></td>
<td>$2/3,1/3,3/2 [0,0,w]$</td>
<td>$2/3,1/3,1/2 [0,0,w]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 c 3</td>
<td>$1/3,2/3,1/4 [0,0,0]$</td>
<td>$2/3,1/3,1/4 [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td>$2/3,1/3,3/4 [0,0,0]$</td>
<td>$1/3,2/3,3/4 [0,0,0]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 b 6m</td>
<td>$0,0,0 [0,0,w]$</td>
<td>$0,0,1/2 [0,0,w]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number</th>
<th>Operation</th>
<th>Special Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 a 6</td>
<td>$0,0,1/4 [0,0,0]$</td>
<td>$0,0,3/4 [0,0,0]$</td>
</tr>
</tbody>
</table>

- **Symmetry of Special Projections**
- **Origin at 0,0,z**
- **Origin at x,0,1/2**
- **Origin at x,x/2,1/2**
Origin at center (6/m1') at 6/mcc1'

Asymmetric unit

\[
\begin{align*}
\text{Vertices} & : & 0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/2,1/2,0 \\
& : & 0,0,1/4 & & 1/2,0,1/4 & & 2/3,1/3,1/4 & & 1/2,1/2,1/4 \\
\end{align*}
\]

Symmetry Operations

(1) 1
(1 | 0,0,0)

(4) 2 0,0,z
(2z | 0,0,0)

(7) 2 x,x,1/4
(2xy | 0,0,1/2)

(10) 2 x,x,1/4
(2z | 0,0,1/2)

(2) 3* 0,0,z
(3z | 0,0,0)

(5) 6* 0,0,z
(6z | 0,0,0)

(8) 2 x,0,1/4
(2z | 0,0,1/2)

(11) 2 x,2x,1/4
(2z | 0,0,1/2)

(3) 3' 0,0,z
(3z' | 0,0,0)

(6) 6' 0,0,z
(6z' | 0,0,0)

(9) 2 0,y,1/4
(2y | 0,0,1/2)

(12) 2 2x,x,1/4
(2z | 0,0,1/2)
Continued

<table>
<thead>
<tr>
<th>Number</th>
<th>Transformation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(13)</td>
<td>(1,0,0)</td>
<td>(1')</td>
</tr>
<tr>
<td></td>
<td>(m')</td>
<td>(14) (3')</td>
</tr>
<tr>
<td>(16)</td>
<td>(c')</td>
<td>(15) (3')</td>
</tr>
<tr>
<td>(19)</td>
<td>(c)</td>
<td>(17) (6')</td>
</tr>
<tr>
<td>(22)</td>
<td>(c)</td>
<td>(18) (6')</td>
</tr>
</tbody>
</table>

For \(1'\) + set

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13); \(1'\).

Positions
Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff Letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 m</td>
<td>11'</td>
<td></td>
</tr>
</tbody>
</table>

Coordinates

<table>
<thead>
<tr>
<th>Number</th>
<th>Transformation</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) y_x-y_z [0,0,0]</td>
<td>(3) x+y_x_z [0,0,0]</td>
</tr>
<tr>
<td>(4) x_y_z [0,0,0]</td>
<td>(5) y_x+y_z [0,0,0]</td>
<td>(6) x-y_x_z [0,0,0]</td>
</tr>
<tr>
<td>(7) y_x_z+1/2 [0,0,0]</td>
<td>(8) x-y_z+1/2 [0,0,0]</td>
<td>(9) x_x+y_z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(10) y_x_z+1/2 [0,0,0]</td>
<td>(11) x+y_y_z+1/2 [0,0,0]</td>
<td>(12) x_x-y_z+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>
(13) $x, y, z [0,0,0]$

(14) $y, x+y, z [0,0,0]$

(15) $x-y, x, z [0,0,0]$

(16) $x, y, z [0,0,0]$

(17) $y, x-y, z [0,0,0]$

(18) $x+y, x, z [0,0,0]$

(19) $y, x, z+1/2 [0,0,0]$

(20) $x+y, y, z+1/2 [0,0,0]$

(21) $x, x-y, z+1/2 [0,0,0]$

(22) $y, x, z+1/2 [0,0,0]$

(23) $x-y, x, z+1/2 [0,0,0]$

(24) $x, x+y, z+1/2 [0,0,0]$

12 l m..1' $x, y, 0 [0,0,0]$

$y, x-y, 0 [0,0,0]$

$x, x+y, 0 [0,0,0]$

$y, x+y, 1/2 [0,0,0]$

$y, x+y, 1/2 [0,0,0]$

12 k ..21' $x, 2x, 1/4 [0,0,0]$

$2x, x, 1/4 [0,0,0]$

$x, 2x, 1/4 [0,0,0]$

$2x, x, 1/4 [0,0,0]$

12 j ..2.1' $x, 0, 1/4 [0,0,0]$

$0, x, 1/4 [0,0,0]$

$x, 0, 1/4 [0,0,0]$

$0, x, 1/4 [0,0,0]$

$0, x, 1/4 [0,0,0]$

$0, x, 1/4 [0,0,0]$

12 i 2..1' $1/2, 0, z [0,0,0]$

$0, 1/2, z [0,0,0]$

$1/2, 1/2, z [0,0,0]$

$0, 1/2, z [0,0,0]$

$1/2, 1/2, z [0,0,0]$

$0, 1/2, z+1/2 [0,0,0]$

$1/2, 1/2, z+1/2 [0,0,0]$

8 h 3..1' $1/3, 2/3, z [0,0,0]$

$2/3, 1/3, z [0,0,0]$

$2/3, 1/3, z+1/2 [0,0,0]$

$1/3, 2/3, z+1/2 [0,0,0]$

$2/3, 1/3, z+1/2 [0,0,0]$

$1/3, 2/3, z+1/2 [0,0,0]$

$2/3, 1/3, z+1/2 [0,0,0]$

6 g 2/m..1' $1/2, 0, 0 [0,0,0]$

$0, 1/2, 0 [0,0,0]$

$1/2, 1/2, 0 [0,0,0]$

$0, 1/2, 1/2 [0,0,0]$

$0, 1/2, 1/2 [0,0,0]$

$1/2, 1/2, 1/2 [0,0,0]$

$0, 1/2, 1/2 [0,0,0]$

6 f 2221' $1/2, 0, 1/4 [0,0,0]$

$0, 1/2, 1/4 [0,0,0]$

$1/2, 1/2, 1/4 [0,0,0]$

$0, 1/2, 3/4 [0,0,0]$

$1/2, 1/2, 3/4 [0,0,0]$

4 e 6..1' $0, 0, z [0,0,0]$

$0, 0, z+1/2 [0,0,0]$

$0, 0, z [0,0,0]$

$0, 0, z+1/2 [0,0,0]$

$0, 0, z+1/2 [0,0,0]$

4 d 6..1' $1/3, 2/3, 0 [0,0,0]$

$2/3, 1/3, 0 [0,0,0]$

$2/3, 1/3, 1/2 [0,0,0]$

$1/3, 2/3, 1/2 [0,0,0]$

$2/3, 1/3, 1/2 [0,0,0]$

$1/3, 2/3, 1/2 [0,0,0]$

4 c 3.21' $1/3, 2/3, 1/4 [0,0,0]$

$2/3, 1/3, 1/4 [0,0,0]$

$2/3, 1/3, 3/4 [0,0,0]$

$2/3, 1/3, 3/4 [0,0,0]$

$1/3, 2/3, 3/4 [0,0,0]$

$1/3, 2/3, 3/4 [0,0,0]$

192.2.1477 - 3 - 3243
Continued 192.2.1477 P6/mcc1′

| 2 b | 6/m..1′ | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] |
| 2 a | 6221′ | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p6mm1′</th>
<th>Along [1,0,0] p2mm1′</th>
<th>Along [2,1,0] p2mm1′</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mathbf{a}^* = \mathbf{a}) (\mathbf{b}^* = \mathbf{b})</td>
<td>(\mathbf{a}^* = \mathbf{c}/2) (\mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2)</td>
<td>(\mathbf{a}^* = \mathbf{c}/2) (\mathbf{b}^* = \mathbf{b}/2)</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
Origin at center (6/m') at 6/m'cc

Asymmetric unit: 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ (1+y)/2; y ≤ min (1-x,x)

Vertices:
- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/2,1/2,0
- 0,0,1/4
- 1/2,0,1/4
- 2/3,1/3,1/4
- 1/2,1/2,1/4

Symmetry Operations:

1. 1
   (1) 3+ 0,0,0
   (2) 3+ 0,0,0
   (3) 3+ 0,0,0
   (4) 2 0,0,0
   (5) 6+ 0,0,0
   (6) 6+ 0,0,0
   (7) 2' x,x,1/4
   (8) 2' x,0,1/4
   (9) 2' 0,y,1/4
   (10) 2' x,x,1/4
   (11) 2' x,2x,1/4
   (12) 2' 2x,x,1/4

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Continued

| (13) | 0,0,0 |
| (14) | 0,0,z |
| (15) | 0,0,0 |

Generators selected

(1); 1(0,0); 1(0,1,0); 1(0,0,1); 2(4); 7(7); 13(13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y,-x,-z [v,-u,-w]</td>
</tr>
<tr>
<td>(4) x+y,z [u-v,w]</td>
<td>(5) y,-x,-z [v,u+v,w]</td>
<td>(6) x-y,z [u-v,u,w]</td>
</tr>
<tr>
<td>(7) y,x,z+1/2 [v,u,w]</td>
<td>(8) x-y,-z+1/2 [v,u+w]</td>
<td>(9) x-y,z+1/2 [u,u+v,w]</td>
</tr>
<tr>
<td>(10) y,x,z+1/2 [v,u,w]</td>
<td>(11) x+y,-z+1/2 [u,u+v,w]</td>
<td>(12) x-y,-z+1/2 [u,u+v,w]</td>
</tr>
<tr>
<td>(13) x+y,z [u,v,w]</td>
<td>(14) y,-x,-z [v,u+v,w]</td>
<td>(15) x+y,z [u+v,u,w]</td>
</tr>
<tr>
<td>(16) x,y,z [u,v,w]</td>
<td>(17) x+y,z [u-v,u,w]</td>
<td>(18) x+y,z [u+v,u,w]</td>
</tr>
<tr>
<td>(19) y,x,z+1/2 [v,u,w]</td>
<td>(20) x+y,y,z+1/2 [u,v+w]</td>
<td>(21) x-y,y,z+1/2 [u,u+v,w]</td>
</tr>
<tr>
<td>(22) y,x,z+1/2 [v,u,w]</td>
<td>(23) x+y,y,z+1/2 [u,v+w]</td>
<td>(24) x+y,z+1/2 [u,u+v,w]</td>
</tr>
</tbody>
</table>

12 l m'.. x,y,0 [u,v,0] y,-x,0 [v,-u,0] x+y,0 [u+v,0] y,x,0 [v,u,0] x+y,0 [u+v,0] x-y,0 [u-v,0] y,x,1/2 [v,0] x+y,1/2 [u+v,0] y-x,1/2 [v,u] x+y,1/2 [u+v,0] x-y,1/2 [u-v,0]

12 k ..2' x,2x,1/4 [u,0,w] 2x,-x,1/4 [0,u,w] x,x,1/4 [u,u] x,1/4 [u,u] 2x,1/4 [0,u] x,x,1/4 [u,u] x,1/4 [u,u] x,1/4 [u,u] x,1/4 [u,u] x,1/4 [u,u] x,1/4 [u,u] x,1/4 [u,u]
Continued

12  j  0.2'.  x,0,1/4 [u,2u,w]  0,x,1/4 [2u, u,w]  x, x,1/4 [u, u,w]
     x,0,1/4 [u,2u,w]  0,x,1/4 [2u,u,w]  x,x,1/4 [u,u,w]
     x,0,3/4 [u,2u,w]  0,x,3/4 [2u,u,\bar{w}]  x,x,3/4 [u,u,\bar{w}]
     x,0,3/4 [u,2u,\bar{w}]  0,x,3/4 [2u, u,\bar{w}]  x, x,3/4 [u, u,\bar{w}]

12  i  2..  1/2,0,z [0,0,w]  0,1/2,z [0,0,w]  1/2,1/2,z [0,0,w]
     0,1/2,z+1/2 [0,0,w]  1/2,0,z+1/2 [0,0,w]  1/2,1/2,z+1/2 [0,0,w]
     1/2,0,z  0,1/2,z  1/2,1/2,z  [0,0,w]  1/2,1/2,z [0,0,w]
     0,1/2,z+1/2 [0,0,w]  1/2,0,z+1/2 [0,0,w]  1/2,1/2,z+1/2 [0,0,w]

8  h  3..  1/3,2/3,z [0,0,w]  2/3,1/3,z [0,0,w]  2/3,1/3,z+1/2 [0,0,w]
     2/3,1/3,z [0,0,\bar{w}]  1/3,2/3,z [0,0,\bar{w}]  1/3,2/3,z+1/2 [0,0,\bar{w}]
     1/3,2/3,z [0,0,w]  2/3,1/3,z+1/2 [0,0,w]  2/3,1/3,z+1/2 [0,0,\bar{w}]

6  g  2/m'.  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]
     0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]
     1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]

6  f  22'2'  1/2,0,1/4 [0,0,w]  0,1/2,1/4 [0,0,w]  1/2,1/2,1/4 [0,0,w]
     1/2,0,3/4 [0,0,w]  0,1/2,3/4 [0,0,w]  1/2,1/2,3/4 [0,0,w]

4  e  6..  0,0,z [0,0,0]  0,0,z+1/2 [0,0,w]  0,0,z [0,0,\bar{w}]  0,0,z+1/2 [0,0,\bar{w}]

4  d  6'..  1/3,2/3,0 [0,0,0]  2/3,1/3,0 [0,0,0]  2/3,1/3,1/2 [0,0,0]
     1/3,2/3,0 [0,0,0]  2/3,1/3,1/2 [0,0,0]  1/3,2/3,1/2 [0,0,0]

4  c  3.2'  1/3,2/3,1/4 [0,0,0]  2/3,1/3,1/4 [0,0,0]  2/3,1/3,3/4 [0,0,\bar{w}]
     1/3,2/3,1/4 [0,0,w]  2/3,1/3,3/4 [0,0,w]  1/3,2/3,3/4 [0,0,\bar{w}]

2  b  6/m'..  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]

2  a  62'2'  0,0,1/4 [0,0,w]  0,0,3/4 [0,0,\bar{w}]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm</th>
<th>Along [1,0,0]</th>
<th>p2m' 2m'm'</th>
<th>Along [2,1,0]</th>
<th>p2a' 2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a  b* = b</td>
<td>a* = c/2  b* = (a + 2b)/2</td>
<td>a* = c/2  b* = b/2</td>
<td>a* = c/2  b* = b/2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0
**Origin** at center (6'/m) at 6'/mc'c

**Asymmetric unit**

- **Vertices**
  - $0,0,0$
  - $1/2,0,0$
  - $2/3,1/3,0$
  - $1/2,1/2,0$
  - $0,0,1/4$
  - $1/2,0,1/4$
  - $2/3,1/3,1/4$
  - $1/2,1/2,1/4$

**Symmetry Operations**

- (1) $1$
  - $(1|0,0,0)$
- (2) $3^+ 0,0,z$
  - $(3_z|0,0,0)$
- (3) $3^- 0,0,z$
  - $(3_z^{-1}|0,0,0)$
- (4) $2' 0,0,z$
  - $(2_z|0,0,0)'$
- (5) $6' 0,0,z$
  - $(6_z^{-1}|0,0,0)'$
- (6) $6^- 0,0,z$
  - $(6_z|0,0,0)'$
- (7) $2 x,x,1/4$
  - $(2_x|0,0,1/2)$
- (8) $2 x,0,1/4$
  - $(2_z|0,0,1/2)$
- (9) $2 y,y,1/4$
  - $(2_y|0,0,1/2)$
- (10) $2' x,0,1/4$
  - $(2_z|0,0,1/2)'$
- (11) $2' x,2x,1/4$
  - $(2_z|0,0,1/2)'$
- (12) $2' 2x,x,1/4$
  - $(2_z|0,0,1/2)'$
Continued

(13) \( \overline{1} \cdot 0,0,0 \)  
\( (\overline{1}|0,0,0') \)  

(14) \( \overline{3} \cdot 0,0,z; 0,0,0 \)  
\( (3|0,0,0') \)  

(15) \( \overline{3} \cdot 0,0,z; 0,0,0 \)  
\( (3|0,0,0') \)  

(16) \( m \ x,y,0 \)  
\( (m|0,0,1/2) \)  

(17) \( 6 \cdot 0,0,z; 0,0,0 \)  
\( (6|0,0,1/2) \)  

(18) \( 6 \cdot 0,0,z; 0,0,0 \)  
\( (6|0,0,1/2) \)  

(19) \( c' (0,0,1/2) \ x,x,z \)  
\( (m_x|0,0,1/2) \)  

(20) \( c' (0,0,1/2) \ x,2x,z \)  
\( (m_x|0,0,1/2) \)  

(21) \( c' (0,0,1/2) \ 2x,x,z \)  
\( (m_y|0,0,1/2) \)  

(22) \( c (0,0,1/2) \ x,x,z \)  
\( (m_z|0,0,1/2) \)  

(23) \( c (0,0,1/2) \ x,0,z \)  
\( (m_z|0,0,1/2) \)  

(24) \( c (0,0,1/2) \ 0,y,z \)  
\( (m_z|0,0,1/2) \)  

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).  

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>24 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) y \cdot x-y,z [v,u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) ( \bar{x},y,z[u,v,w] )</td>
<td>(5) y,( \bar{x}+y,z[u,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 ( [v,u,w] )</td>
<td>(8) x-y,( \bar{y},z+1/2[u-v,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(10) ( \bar{y},x,z+1/2[v,u,w] )</td>
<td>(11) ( \bar{x}+y,\bar{z}+1/2[u-v,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(13) ( \bar{x},\bar{y},z[u,v,w] )</td>
<td>(14) ( \bar{y}+x,\bar{z}[v,\bar{u}+v,w] )</td>
</tr>
<tr>
<td></td>
<td>(16) ( \bar{x},\bar{y},\bar{z}[u,v,w] )</td>
<td>(17) ( y,\bar{x}+y,\bar{z}[v,\bar{u}+v,w] )</td>
</tr>
<tr>
<td></td>
<td>(19) ( y,\bar{x},z+1/2[v,\bar{u},w] )</td>
<td>(20) ( \bar{y}+x+y,\bar{z}+1/2[u+v,v,w] )</td>
</tr>
<tr>
<td></td>
<td>(22) ( y,x,z+1/2[v,\bar{u},w] )</td>
<td>(23) ( \bar{y}+x+y,\bar{z}+1/2[u+v,v,w] )</td>
</tr>
</tbody>
</table>

12 l m.. 
| x,y,0 \( [0,0,w] \) | \( \bar{y},x-y,0[0,0,w] \) | \( x+y,x,0[0,0,w] \) |
| \( \bar{x},y,0[0,0,w] \) | y,\( x+y,0[0,0,w] \) | x-y,x,0 \( [0,0,w] \) |
| y,x,1/2 \( [0,0,w] \) | x-y,\( \bar{y},1/2[0,0,w] \) | \( x,\bar{x}+y,1/2[0,0,w] \) |
| \( \bar{y},x,1/2[0,0,w] \) | \( \bar{x}+y,y,1/2[0,0,w] \) | x-x-y,1/2 \( [0,0,w] \) |

12 k \( .2' \) 
| x,2x,1/4 \( [u,0,w] \) | \( 2\bar{x},x,1/4[0,u,w] \) | \( \bar{x},1/4[u,u,w] \) |
| \( \bar{x},2\bar{x},1/4[0,u,\bar{w}] \) | \( 2\overline{x},x,1/4[0,u,\bar{w}] \) | \( \bar{x},1/4[u,\bar{u},w] \) |
| \( \bar{x},2\bar{x},3/4[u,0,w] \) | \( 2\overline{x},x,3/4[0,\bar{u},w] \) | \( \bar{x},3/4[u,u,\bar{w}] \) |
| x,2x,3/4 \( [0,u,\bar{w}] \) | \( 2\bar{x},x,3/4[0,u,w] \) | \( x,3/4[u,u,\bar{w}] \) |
Symmetry of Special Projections

Along [0,0,1] p6mm1'  
\( \text{a}^* = \text{a} \quad \text{b}^* = \text{b} \)  
Origin at 0,0,0

Along [1,0,0] p2mm  
\( \text{a}^* = \text{c}/2 \quad \text{b}^* = (\text{a} + 2\text{b})/2 \)  
Origin at x,0,0

Along [2,1,0] p2a,2mm  
\( \text{a}^* = \text{c}/2 \quad \text{b}^* = \text{b}/2 \)  
Origin at x,x/2,0

\begin{align*}
12 & j \text{  .2.} & x,0,1/4 [u,0,0] & 0,x,1/4 [0,u,0] & x,x,1/4 [u,0,0] \\
& & x,0,1/4 [u,0,0] & 0,x,1/4 [0,u,0] & x,x,1/4 [u,0,0] \\
& & x,0,3/4 [u,0,0] & 0,x,3/4 [0,u,0] & x,x,3/4 [u,u,0] \\
& & x,0,3/4 [u,0,0] & 0,x,3/4 [0,u,0] & x,x,3/4 [u,u,0] \\
12 & i \text{  2'.} & 1/2,0,z [u,v,0] & 0,1/2,z [v,u-v,0] & 1/2,1/2,z [u+v,u,0] \\
& & 0,1/2,z+1/2 [v,u,0] & 1/2,0,z+1/2 [u-v,v,0] & 1/2,1/2,z+1/2 [u,u+v,0] \\
& & 0,1/2,z [u,v,0] & 1/2,0,z [v,u+v,0] & 1/2,1/2,z [u-u+v,0] \\
& & 0,1/2,z+1/2 [v,u,0] & 1/2,0,z+1/2 [u+v,v,0] & 1/2,1/2,z+1/2 [u,u-v,0] \\
8 & h \text{  3..} & 1/3,2/3,z [0,0,w] & 2/3,1/3,z [0,0,w] & 2/3,1/3,z+1/2 [0,0,w] \\
& & 2/3,1/3,z [0,0,w] & 1/3,2/3,z [0,0,w] & 1/3,2/3,z+1/2 [0,0,w] \\
6 & g \text{  2'm..} & 1/2,0,0 [0,0,0] & 0,1/2,0 [0,0,0] & 1/2,1/2,0 [0,0,0] \\
& & 0,1/2,1/2 [0,0,0] & 1/2,0,1/2 [0,0,0] & 1/2,1/2,1/2 [0,0,0] \\
6 & f \text{  2'22'} & 1/2,0,1/4 [u,0,0] & 0,1/2,1/4 [u,0,0] & 1/2,1/2,1/4 [u,0,0] \\
& & 1/2,0,3/4 [u,0,0] & 0,1/2,3/4 [u,0,0] & 1/2,1/2,3/4 [u,0,0] \\
4 & e \text{  6..} & 0,0,0 [0,0,0] & 0,0,0 [0,0,0] & 0,0,0 [0,0,0] \\
& & 0,0,0 [0,0,0] & 0,0,0 [0,0,0] & 0,0,z+1/2 [0,0,0] \\
4 & d \text{  6..} & 1/3,2/3,0 [0,0,w] & 2/3,1/3,0 [0,0,w] & 1/3,2/3,1/2 [0,0,w] \\
& & 2/3,1/3,0 [0,0,w] & 1/3,2/3,1/2 [0,0,w] & 1/3,2/3,1/2 [0,0,w] \\
4 & c \text{  3.2'} & 1/3,2/3,1/4 [0,0,w] & 2/3,1/3,1/4 [0,0,w] & 1/3,2/3,3/4 [0,0,w] \\
& & 2/3,1/3,1/4 [0,0,w] & 1/3,2/3,3/4 [0,0,w] & 1/3,2/3,3/4 [0,0,w] \\
2 & b \text{  6'm..} & 0,0,0 [0,0,0] & 0,0,0 [0,0,0] & 0,0,1/2 [0,0,0] \\
2 & a \text{  6'22'} & 0,0,1/4 [0,0,0] & 0,0,1/4 [0,0,0] & 0,0,3/4 [0,0,0]
Origin at center (6'/m) at 6'/mcc'

Asymmetric unit

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ (1+y)/2; y ≤ min (1-x,x)

Vertices

0,0,0 1/2,0,0 2/3,1/3,0 1/2,1/2,0
0,0,1/4 1/2,0,1/4 2/3,1/3,1/4 1/2,1/2,1/4

Symmetry Operations

(1) 1
(1 0,0,0)

(4) 2' 0,0,z
(2z 0,0,0)'

(7) 2' x,x,1/4
(2x 0,0,1/2)'

(10) 2 x,x,1/4
(2 0,0,1/2)

(2) 3* 0,0,z
(3z 0,0,0)

(5) 6' 0,0,z
(6z 0,0,0)'

(8) 2' x,0,1/4
(2z 0,0,1/2)'

(11) 2 x,2x,1/4
(2z 0,0,1/2)

(3) 3' 0,0,z
(3z 0,0,0)

(6) 6' 0,0,z
(6z 0,0,0)'

(9) 2' 0,y,1/4
(2y 0,0,1/2)'

(12) 2 2x,x,1/4
(2 0,0,1/2)
Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 m 1  (1) x,y,z [u,v,w]  
(4) $\bar{x}, \bar{y},z$ [u,v,w]  
(7) y,x,z+1/2 [v,u,w]  
(10) $\bar{y}, \bar{x},z+1/2$ [v,u,w]  
(13) $x, \bar{y},z$ [u,\bar{v},w]  
(16) x,y,z [u,\bar{v},w]  
(19) $\bar{y}, \bar{x},z+1/2$ [v,u,w]  
(22) y,x,z+1/2 [v,u,w]  

12 l m.. x,y,0 [0,0,w]  
$\bar{x}, y,0$ [0,0,w]  
$x, y,1/2$ [0,0,w]  
$\bar{y}, \bar{x},1/2$ [0,0,w]  

12 k ..2 x,2x,1/4 [u,2u,0]  
$\bar{x},2\bar{x},1/4$ [u,2u,0]  
$x,2x,3/4$ [u,2u,0]  
$\bar{x},2\bar{x},3/4$ [u,2u,0]  
$x,2x,3/4$ [u,2u,0]  

Continued

(13) $\bar{1}$ 0,0,0  
(14) $\bar{3}$+ 0,0,z; 0,0,0  
(15) $\bar{3}$+ 0,0,z; 0,0,0  

(16) m x,y,0  
(17) $\bar{6}$ 0,0,z; 0,0,0  
(18) $\bar{6}$ 0,0,z; 0,0,0  

(19) c (0,0,1/2) x,\bar{x},z  
(20) c (0,0,1/2) x,2x,z  
(21) c (0,0,1/2) 2x,x,z  

(22) $c'$(0,0,1/2) x,x,z  
(23) $c'$(0,0,1/2) x,0,z  
(24) $c'$(0,0,1/2) 0,y,z  

12 l m.. x,y,0 [0,0,w]  
$\bar{x}, y,0$ [0,0,w]  
$x, y,1/2$ [0,0,w]  
$\bar{y}, \bar{x},1/2$ [0,0,w]  

12 k ..2 x,2x,1/4 [u,2u,0]  
$\bar{x},2\bar{x},1/4$ [u,2u,0]  
$x,2x,3/4$ [u,2u,0]  
$\bar{x},2\bar{x},3/4$ [u,2u,0]  
$x,2x,3/4$ [u,2u,0]  

Generators selected  

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).
Continued

192.5.1480

P6'/mcc'

12 j 2'. x,0,1/4 [u,2u,w] 0,x,1/4 [2u, u,w] x,x,1/4 [u, u,w]
   x,0,1/4 [u,2u,w] 0,x,1/4 [2u, u,w] x,x,1/4 [u, u,w]
   x,0,3/4 [u,2u,w] 0,x,3/4 [2u, u,w] x,x,3/4 [u, u,w]
   x,0,3/4 [u,2u,w] 0,x,3/4 [2u, u,w] x,x,3/4 [u, u,w]

12 i 2'.. 1/2,0,z [u,v,0] 0,1/2,z [v,u-v,0] 1/2,1/2,z [u+v,u,0]
   0,1/2,z+1/2 [v, u,0] 1/2,0,z+1/2 [u+v,v,0] 1/2,1/2,z+1/2 [u,u-v,0]
   1/2,0,z [u,v,0] 0,1/2,z [v,u-v,0] 1/2,1/2,z [u-u+v,0]
   0,1/2,z+1/2 [v,u,0] 1/2,0,z+1/2 [u-v,v,0] 1/2,1/2,z+1/2 [u+u+v,0]

8 h 3.. 1/3,2/3,z [0,0,w] 2/3,1/3,z [0,0,0] 2/3,1/3,z [0,0,0] 1/3,2/3,z+1/2 [0,0,0]
   2/3,1/3,z [0,0,w] 1/3,2/3,z [0,0,w] 1/3,2/3,z+1/2 [0,0,0] 2/3,1/3,z+1/2 [0,0,w]

6 g 2/m.. 1/2,0,0 [0,0,0] 0,1/2,0 [0,0,0] 1/2,1/2,0 [0,0,0]
   0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,1/2,1/2 [0,0,0]

6 f 2'2'1 1/2,0,1/4 [u,2u,0] 0,1/2,1/4 [2u, u,0] 1/2,1/2,1/4 [u, u,0]
   1/2,0,3/4 [u,2u,0] 0,1/2,3/4 [2u, u,0] 1/2,1/2,3/4 [u, u,0]

4 e 6.. 0,0,z [0,0,0] 0,0,z+1/2 [0,0,0] 0,0,z+1/2 [0,0,0] 0,0,z+1/2 [0,0,0]

4 d 6.. 1/3,2/3,0 [0,0,w] 2/3,1/3,0 [0,0,0] 2/3,1/3,1/2 [0,0,w] 1/3,2/3,1/2 [0,0,w]

4 c 3.2 1/3,2/3,1/4 [0,0,0] 2/3,1/3,1/4 [0,0,0] 2/3,1/3,3/4 [0,0,0] 1/3,2/3,3/4 [0,0,0]

2 b 6/m.. 0,0,0 [0,0,0] 0,0,1/2 [0,0,0]

2 a 6'2'2 0,0,1/4 [0,0,0] 0,0,3/4 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm1'</th>
<th>Along [1,0,0]</th>
<th>p_{cc} 2mm</th>
<th>Along [2,1,0]</th>
<th>p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a^* = a</td>
<td>b^* = b</td>
<td>a^* = c/2</td>
<td>b^* = (a + 2b)/2</td>
<td>a^* = c/2</td>
<td>b^* = b/2</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td>Origin at x,x/2,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at center (6'/m') at 6'/m'c'c

**Asymmetric unit**

- 0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ (1+y)/2; y ≤ min (1-x, x)

**Vertices**

- 0,0,0
- 1/2,0,0
- 2/3,1/3,0
- 1/2,1/2,0
- 0,0,1/4
- 1/2,0,1/4
- 2/3,1/3,1/4
- 1/2,1/2,1/4

**Symmetry Operations**

1. 1
   - (1, 0, 0, 0)
2. 3* 0,0,z
   - (3z, 0,0,0)
3. 3* 0,0,z
   - (3z, 0,0,0)
4. 2' 0,0,z
   - (2z, 0,0,0)'
   - 6' - 0,0,z
   - (6z, 0,0,0)'
5. 6' - 0,0,z
   - (6z, 0,0,0)'
6. 6' - 0,0,z
   - (6z, 0,0,0)'
7. 2' x,x,1/4
   - (2x, 0,0,1/2)'
8. 2' x,0,1/4
   - (2x, 0,0,1/2)'
9. 2' 0,y,1/4
   - (2z, 0,0,1/2)'
10. 2 x,x,1/4
    - (2x, 0,0,1/2)
11. 2 x,2x,1/4
    - (2x, 0,0,1/2)
12. 2 2x,x,1/4
    - (2x, 0,0,1/2)
Continued

192.6.1481 P6'/m'c'c

(13) 0,0,0  (14) 0,0,z; 0,0,0  (15) 0,0,z; 0,0,0
(16) m' x,y,0 (17) 0,0,z; 0,0,0  (18) 0,0,z; 0,0,0
(m'|0,0,1/2') (19) c' (0,0,1/2)  (20) c' (0,0,1/2)
(m'|0,0,1/2') (21) c' (0,0,1/2)  (22) c' (0,0,1/2)
(m'|0,0,1/2') (23) c' (0,0,1/2)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
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<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(5) y,x+y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x-y,x,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
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<td>(9) x,x+y,z+1/2 [u,u-v,w]</td>
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<td>(10) y,x,z+1/2 [v,u,w]</td>
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<td>(11) x+y,x,z+1/2 [u+v,u,w]</td>
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<tr>
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<td>(12) x,x+y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(13) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(14) y,x+y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(15) x-y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(16) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(17) y,x+y,z [v,u-v,w]</td>
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<tr>
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<td>(18) x+y,x,z [u+v,u,w]</td>
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<td></td>
<td>(19) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(20) x+y,x,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(21) x,x+y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(22) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(23) x-y,x,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(24) x,x+y,z+1/2 [u,u-v,w]</td>
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</tbody>
</table>

12 l m'.

<table>
<thead>
<tr>
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<th>Coordinates</th>
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<tbody>
<tr>
<td>12 l m'.</td>
<td>x,y,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,0 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,1/2 [v,u,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,1/2 [v,u,0]</td>
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<td></td>
<td>x,y,1/2 [u+v,v,0]</td>
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<tr>
<td></td>
<td>x,y,1/2 [u+v,v,0]</td>
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</tbody>
</table>

12 k .2

<table>
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<th>Coordinates</th>
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<tbody>
<tr>
<td>12 k .2</td>
<td>x,2x,1/4 [u,2u,0]</td>
</tr>
<tr>
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<td>x,2x,1/4 [u,2u,0]</td>
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<td></td>
<td>x,2x,3/4 [u,2u,0]</td>
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<tr>
<td></td>
<td>x,2x,3/4 [u,2u,0]</td>
</tr>
</tbody>
</table>

192.6.1481 - 2 - 3255
Symmetry of Special Projections

Along \([0,0,1]\) \(p6\overline{m}'m\)  \(p6\overline{m}'m\)  \(p2\overline{m}'mm'\) \(p2\overline{m}'mm'\)  \(p_{2\overline{a}}2mm\) \\
a* = \(a\)  \(b* = b\)  \(a* = (a + 2b)/2\)  \(b* = c/2\)  \(a* = c/2\)  \(b* = b/2\)  \\
Origin at 0,0,z  \(\text{Origin at } x,0,0\)  \(\text{Origin at } x,x/2,1/4\)
**Origin** at center (6'/m') at 6'/m'cc'

**Asymmetric unit**

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 2/3;</td>
<td>0 ≤ y ≤ 1/2;</td>
<td>0 ≤ z ≤ 1/4;</td>
</tr>
</tbody>
</table>

**Vertices**

<table>
<thead>
<tr>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>2/3,1/3,0</th>
<th>1/2,1/2,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
<td>2/3,1/3,1/4</td>
<td>1/2,1/2,1/4</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. 1
   
2. 3' 0,0,z
   
3. 3' 0,0,z
   
4. 2' 0,0,z
   
5. 6' 0,0,0
   
6. 6' 0,0,0
   
7. 2 x,x,1/4
   
8. 2' 0,0,1/4
   
9. 2 0,y,1/4
   
10. 2' x,x,1/4
    
11. 2' x,2x,1/4
    
12. 2' 2x,x,1/4
Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Generators selected (1): t(1,0,0); t(0,1,0); t(0,0,1); (2): (4); (7): (13).

Coordinates

Continued

\[
\begin{align*}
(13) & \quad \bar{1} \quad 0,0,0 \\
(14) & \quad \bar{3}^+ \quad 0,0,z; \quad 0,0,0 \\
(15) & \quad \bar{3}^- \quad 0,0,0; \quad 0,0,0 \\
(16) & \quad m' \quad x,y,0 \\
(17) & \quad \bar{6}^- \quad 0,0,z; \quad 0,0,0 \\
(18) & \quad \bar{6}^+ \quad 0,0,0; \quad 0,0,0 \\
(19) & \quad c \quad (0,0,1/2) \\
(20) & \quad c \quad (0,0,1/2) \\
(21) & \quad c \quad (0,0,1/2) \\
(22) & \quad c' \quad (0,0,1/2) \\
(23) & \quad c' \quad (0,0,1/2) \\
(24) & \quad c' \quad (0,0,1/2) \\
\end{align*}
\]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>12</th>
<th>i</th>
<th>$2''$</th>
<th>$x,0,1/4$</th>
<th>$0,x,1/4$</th>
<th>$x,x,1/4$</th>
<th>$x,x,3/4$</th>
<th>$0,x,3/4$</th>
<th>$x,x,3/4$</th>
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</thead>
<tbody>
<tr>
<td>12</td>
<td>j</td>
<td>$2''$</td>
<td>$1/2,z$</td>
<td>$0,1/2,z$</td>
<td>$1/2,1/2,z$</td>
<td>$1/2,1/2,z$</td>
<td>$0,1/2,z$</td>
<td>$1/2,1/2,z$</td>
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<tr>
<td>8</td>
<td>h</td>
<td>$3'$</td>
<td>$1/3,2/3,z$</td>
<td>$2/3,1/3,z$</td>
<td>$1/3,2/3,z+1/2$</td>
<td>$1/3,2/3,z+1/2$</td>
<td>$2/3,1/3,z+1/2$</td>
<td>$1/3,2/3,z+1/2$</td>
</tr>
<tr>
<td>6</td>
<td>g</td>
<td>$2''$</td>
<td>$2/3,0,0$</td>
<td>$1/2,2,1/2$</td>
<td>$1/2,1/2,2$</td>
<td>$1/2,1/2,2$</td>
<td>$2/3,0,0$</td>
<td>$1/2,2,1/2$</td>
</tr>
<tr>
<td>6</td>
<td>f</td>
<td>$2''$</td>
<td>$0,1/2,1/4$</td>
<td>$1/2,1/2,1/4$</td>
<td>$1/2,1/2,1/4$</td>
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<td>4</td>
<td>e</td>
<td>$6'$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
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<td>$0,0,0$</td>
<td>$0,0,0$</td>
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<tr>
<td>4</td>
<td>d</td>
<td>$6'$</td>
<td>$1/3,2/3,0$</td>
<td>$2/3,1/3,0$</td>
<td>$2/3,1/3,1/2$</td>
<td>$2/3,1/3,1/2$</td>
<td>$1/3,2/3,1/2$</td>
<td>$2/3,1/3,1/2$</td>
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<tr>
<td>4</td>
<td>c</td>
<td>$3'$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
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<td>2</td>
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<td>$0,0,0$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
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</tbody>
</table>

### Symmetry of Special Projections (continued)

- **Along $[0,0,1]$** $p6'm'm'$
- **Along $[1,0,0]$** $p_{2/m}2'm'm$
- **Along $[2,1,0]$** $p2'm'm$

<table>
<thead>
<tr>
<th>$a^*$</th>
<th>$a^*$</th>
<th>$b^*$</th>
<th>$b^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = a$</td>
<td>$a^* = b$</td>
<td>$a^* = c/2$</td>
<td>$a^* = b$</td>
</tr>
<tr>
<td>$b^* = b$</td>
<td>$b^* = (a + 2b)/2$</td>
<td>$b^* = c/2$</td>
<td>$b^* = c/2$</td>
</tr>
<tr>
<td>Origin at $0,0,z$</td>
<td>Origin at $x,0,1/4$</td>
<td>Origin at $x,0,1/4$</td>
<td>Origin at $x,x/2,0$</td>
</tr>
</tbody>
</table>
Origin at center (6/m) at 6/mc'c'

Asymmetric unit

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; x ≤ (1+y)/2; y ≤ min (1-x,x)

Vertices

0,0,0 1/2,0,0 2/3,1/3,0 1/2,1/2,0
0,0,1/4 1/2,0,1/4 2/3,1/3,1/4 1/2,1/2,1/4

Symmetry Operations

(1) 1
(1) 1

(2) 3z 0,0,z
(3) 3z 0,0,z

(3 z) 0,0,0

(4) 2 0,0,z
(2z 0,0,0)

(5) 6z 0,0,z
(6z 0,0,0)

(6) 6z 0,0,1/2')

(7) 2z x,x,1/4
(2z 0,0,1/2')

(8) 2z x,0,1/4
(2z 0,0,1/2')

(9) 2z 0,y,1/4
(2z 0,0,1/2')

(10) 2z x,x,1/4
(2z 0,0,1/2')

(11) 2z x,2x,1/4
(2z 0,0,1/2')

(12) 2z 2x,x,1/4
(2z 0,0,1/2')
Continued

(13) $\bar{1}$ 0,0,0  
(14) $\bar{3}^*$ 0,0,z; 0,0,0  
(15) $\bar{3}^*$ 0,0,z; 0,0,0

(16) m x,y,0  
(m, | 0,0,1/2)

(17) $\bar{6}^*$ 0,0,z; 0,0,0  
(18) $\bar{6}^*$ 0,0,z; 0,0,0

(19) c' (0,0,1/2)  
(m, | 0,0,1/2)'

(20) c' (0,0,1/2)  
(m, | 0,0,1/2)'

(21) c' (0,0,1/2)  
(m, | 0,0,1/2)'

(22) c' (0,0,1/2)  
(m, | 0,0,1/2)'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, 
Wyckoff letter, 
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 m 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x-y,z [v,u-v,w]</td>
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<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(5) y, x+y,z [v, u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x-y,x,z [u-v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v, u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x-y, y,z+1/2 [u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x-x, y,z+1/2 [u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) y, x, z+1/2 [v, u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x+y, y, z+1/2 [u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x-x, y, z+1/2 [u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(13) x, y, z [u, v, w]</td>
</tr>
<tr>
<td></td>
<td>(14) y, x+y, z [v, u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(15) x+y, x, z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(16) x, y, z [u, v, w]</td>
</tr>
<tr>
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<td>(17) y, x+y, z [v, u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(18) x+y, x, z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(19) y, x, z+1/2 [v, u,w]</td>
</tr>
<tr>
<td></td>
<td>(20) x+y, y, z+1/2 [u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(21) x-x, y, z+1/2 [u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(22) y, x, z+1/2 [v, u,w]</td>
</tr>
<tr>
<td></td>
<td>(23) x-y, y, z+1/2 [u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(24) x-x, y, z+1/2 [u+v,w]</td>
</tr>
</tbody>
</table>

| 12 l m.. | x,y,0 [0,0,w] |
|          | y,x,0 [0,0,w] |
|          | y,x,1/2 [0,0,w] |
|          | y,x,1/2 [0,0,w] |

| 12 k ..2' | x,2x,1/4 [u,0,w] |
|           | x,2x,1/4 [u,0,w] |
|           | x,2x,3/4 [u,0,w] |

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| 12 | j | 2' | x,0,1/4 [u,2u,w] | 0,x,1/4 [2u, u,w] | x,x,1/4 [u, u,w] |
|    |   |    | x,0,1/4 [u,2u,w] | 0,x,1/4 [2u,u,w] | x,x,1/4 [u,u,w] |
|    |   |    | x,0,3/4 [u,2u,w] | 0,x,3/4 [2u, u,w] | x,x,3/4 [u, u,w] |
|    |   |    | x,0,3/4 [u,2u,w] | 0,x,3/4 [2u,u,w] | x,x,3/4 [u,u,w] |
| 12 | i | 2..| 1/2,0, z [0,0,w] | 0,1/2, z [0,0,w] | 1/2,1/2, z [0,0,w] |
|    |   |    | 0,1/2, z+1/2 [0,0,w] | 1/2,0, z+1/2 [0,0,w] | 1/2,1/2, z+1/2 [0,0,w] |
|    |   |    | 1/2,0, z [0,0,w] | 0,1/2, z [0,0,w] | 1/2,1/2, z [0,0,w] |
|    |   |    | 0,1/2, z+1/2 [0,0,w] | 1/2,0, z+1/2 [0,0,w] | 1/2,1/2, z+1/2 [0,0,w] |
| 8  | h | 3..| 1/3,2/3, z [0,0,w] | 2/3,1/3, z [0,0,w] | 2/3,1/3, z+1/2 [0,0,w] |
|    |   |    | 2/3,1/3, z [0,0,w] | 1/3,2/3, z [0,0,w] | 1/3,2/3, z+1/2 [0,0,w] |
|    |   |    | 2/3,1/3, z [0,0,w] | 1/3,2/3, z+1/2 [0,0,w] | 2/3,1/3, z+1/2 [0,0,w] |
| 6  | g | 2/m..| 1/2,0,0 [0,0,w] | 0,1/2,0 [0,0,w] | 1/2,1/2,0 [0,0,w] |
|    |   |    | 0,1/2,1/2 [0,0,w] | 1/2,0,1/2 [0,0,w] | 1/2,1/2,1/2 [0,0,w] |
| 6  | f | 22'2' | 1/2,0,1/4 [0,0,w] | 0,1/2,1/4 [0,0,w] | 1/2,1/2,1/4 [0,0,w] |
|    |   |    | 1/2,0,3/4 [0,0,w] | 0,1/2,3/4 [0,0,w] | 1/2,1/2,3/4 [0,0,w] |
| 4  | e | 6.. | 0,0, z [0,0,w] | 0,0, z+1/2 [0,0,w] | 0,0, z [0,0,w] |
|    |   |    | 0,0, z [0,0,w] | 0,0, z+1/2 [0,0,w] | 0,0, z+1/2 [0,0,w] |
| 4  | d | 6.. | 1/3,2/3,0 [0,0,w] | 2/3,1/3,0 [0,0,w] | 2/3,1/3,1/2 [0,0,w] |
|    |   |    | 2/3,1/3,0 [0,0,w] | 2/3,1/3,1/2 [0,0,w] | 1/3,2/3,1/2 [0,0,w] |
| 4  | c | 3.2' | 1/3,2/3,1/4 [0,0,w] | 2/3,1/3,1/4 [0,0,w] | 2/3,1/3,3/4 [0,0,w] |
|    |   |    | 2/3,1/3,1/4 [0,0,w] | 2/3,1/3,3/4 [0,0,w] | 1/3,2/3,3/4 [0,0,w] |
| 2  | b | 6/m.. | 0,0,0 [0,0,w] | 0,0,1/2 [0,0,w] | 0,0,1/2 [0,0,w] |
| 2  | a | 62'2' | 0,0,1/4 [0,0,w] | 0,0,3/4 [0,0,w] | 0,0,3/4 [0,0,w] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm1'</th>
<th>Along [1,0,0]</th>
<th>p2'mm'</th>
<th>Along [2,1,0]</th>
<th>p2'mm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = c/2</td>
<td>b* = (a + 2b)/2</td>
<td>a* = c/2</td>
<td>b* = b/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,z Origin at x,0,0 Origin at x,x/2,0
**Origin** at center (6/m') at 6/m'c'c'

**Asymmetric unit**

- $0 \leq x \leq 2/3$
- $0 \leq y \leq 1/2$
- $0 \leq z \leq 1/4$
- $x \leq (1+y)/2$
- $y \leq \min (1-x, x)$

**Vertices**

- $0,0,0$
- $1/2,0,0$
- $2/3,1/3,0$
- $1/2,1/2,0$
- $0,0,1/4$
- $1/2,0,1/4$
- $2/3,1/3,1/4$
- $1/2,1/2,1/4$

**Symmetry Operations**

1. $1$
2. $3^*$ $0,0,z$
3. $3^*$ $0,0,z$
4. $2$ $0,0,z$
5. $6^*$ $0,0,z$
6. $6^*$ $0,0,z$
7. $2x,x,1/4$
8. $2^*$ $x,0,1/4$
9. $2^*$ $0,y,1/4$
10. $2^*$ $x,x,1/4$
11. $2^*$ $x,2x,1/4$
12. $2^*$ $2x,x,1/4$

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<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).</td>
<td>(1) $x$, $y$; $z$</td>
</tr>
<tr>
<td>Positions</td>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
</tr>
<tr>
<td>24</td>
<td>m</td>
</tr>
<tr>
<td></td>
<td>(4) $x$, $y$, $z$ [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) $y$, $x$, $z$ [v,u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) $y$, $x$, $z$ [u,v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(13) $x$, $y$, $z$ [u,v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(16) $x$, $y$, $z$ [u,v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(19) $y$, $x$, $z$ [v,u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(22) $y$, $x$, $z$ [u,v,v,w]</td>
</tr>
<tr>
<td>12</td>
<td>m'</td>
</tr>
<tr>
<td></td>
<td>(4) $x$, $y$, $0$ [u+v,u,0]</td>
</tr>
<tr>
<td></td>
<td>(7) $y$, $x$, $1/2$ [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(10) $y$, $x$, $1/2$ [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(13) $x$, $y$, $1/2$ [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(16) $x$, $y$, $1/2$ [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(19) $x$, $y$, $1/2$ [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>(22) $x$, $y$, $1/2$ [u,v,0]</td>
</tr>
<tr>
<td>12 j .2</td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/4 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [u,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,3/4 [u,0,0]</td>
</tr>
<tr>
<td>12 i 2..</td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,z+1/2 [0,0,w]</td>
</tr>
<tr>
<td>8 h 3..</td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>2/3,1/3,z [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>1/3,2/3,z [0,0,w]</td>
</tr>
<tr>
<td>6 g 2/m'</td>
<td>1/2,0,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>0,1/2,1/2 [0,0,w]</td>
</tr>
<tr>
<td>6 f 222</td>
<td>1/2,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 e 6..</td>
<td>0,0,z [0,0,w]</td>
</tr>
<tr>
<td>4 d 6'</td>
<td>1/3,2,3,0 [0,0,0]</td>
</tr>
<tr>
<td>4 c 3.2</td>
<td>1/3,2,3,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2 b 6/m'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td>2 a 622</td>
<td>0,0,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**: \( p6m'm' \)
  - \( a^* = a \  b^* = b \)
  - Origin at 0,0,z

- **Along [1,0,0]**: \( p2m'm' \)
  - \( a^* = c/2 \  b^* = (a + 2b)/2 \)
  - Origin at x,0,0

- **Along [2,1,0]**: \( p2m'm' \)
  - \( a^* = c/2 \  b^* = b/2 \)
  - Origin at x,x/2,0

---

192.9.1484 - 3 - 3265
Origin at center (31m) at \(\overline{3}c2/m\)

Asymmetric unit

\[
\begin{align*}
0 \leq x &\leq \frac{2}{3}; & 0 \leq y &\leq \frac{1}{2}; & 0 \leq z &\leq \frac{1}{4}; & x &\leq \frac{1+y}{2}; & y &\leq \min (1-x,x)
\end{align*}
\]

Vertices

\[
\begin{align*}
0,0,0 & & 1/2,0,0 & & 2/3,1/3,0 & & 1/2,1/2,0 \\
0,0,1/4 & & 1/2,0,1/4 & & 2/3,1/3,1/4 & & 1/2,1/2,1/4
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & & 1 & & (2) & & 3^+ & & 0,0,z & & (3) & & 3^- & & 0,0,z \\
(1) & & 0,0,0 & & (3z) & & 0,0,0 & & (3z^-1) & & 0,0,0
\end{align*}
\]

\[
\begin{align*}
(4) & & 2 & & (0,0,1/2) & & 0,0,z & & (5) & & 6^- & & (0,0,1/2) & & 0,0,z \\
(2z) & & 0,0,1/2 & & (6z^-1) & & 0,0,1/2 & & (6z^-1) & & 0,0,1/2
\end{align*}
\]

\[
\begin{align*}
(7) & & 2 & & x,x,1/4 & & (8) & & 2 & & x,0,1/4 & & (9) & & 2 & & 0,y,1/4 \\
(2\overline{y}) & & 0,0,1/2 & & (2z) & & 0,0,1/2 & & (2\overline{y}) & & 0,0,1/2 & & (2\overline{y}) & & 0,0,1/2
\end{align*}
\]

\[
\begin{align*}
(10) & & 2 & & \overline{x},\overline{x},0 & & (11) & & 2 & & \overline{x},2\overline{x},0 & & (12) & & 2 & & 2x,x,0 \\
(2\overline{z}) & & 0,0,0 & & (2\overline{z}) & & 0,0,0 & & (2\overline{z}) & & 0,0,0 & & (2\overline{z}) & & 0,0,0
\end{align*}
\]
Continued

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(13) 100,0</td>
<td>(14) 3+ 0,0,0; 0,0,0</td>
<td>(15) 3- 0,0,0; 0,0,0</td>
</tr>
<tr>
<td>(16) m x,y,1/4</td>
<td>(17) 6- 0,0,0; 0,0,1/4</td>
<td>(18) 6+ 0,0,0; 0,0,1/4</td>
</tr>
<tr>
<td>(19) c (0,0,1/2) x,x,z</td>
<td>(20) c (0,0,1/2) x,2x,z</td>
<td>(21) c (0,0,1/2) 2x,x,z</td>
</tr>
<tr>
<td>(22) m x,x,z</td>
<td>(23) m x,0,z</td>
<td>(24) m 0,y,z</td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).
Continued

12  i  ..2  x,2x,0 [u,2u,0]  2x,x,0 [2u, u,0]  x,x,0 [u, u,0]
     x,2x,1/2 [u,2u,0]  2x,x,1/2 [2u,u,0]  x,x,1/2 [u,u,0]
     x,2x,0 [u,2u,0]  2x,x,0 [2u,u,0]  x,x,0 [u,u,0]
     x,2x,1/2 [u,2u,0]  2x,x,1/2 [2u,u,0]  x,x,1/2 [u,u,0]

8  h  3..  1/3,2/3,z [0,0,w]  2/3,1/3,z+1/2 [0,0,w]  2/3,1/3,z [0,0,w]  1/3,2/3,z [0,0,w]
     2/3,1/3,z [0,0,w]  1/3,2/3,z+1/2 [0,0,w]  1/3,2/3,z+1/2 [0,0,w]  2/3,1/3,z [0,0,w]

6  g  m2m  x,0,1/4 [0,0,0]  0,x,1/4 [0,0,0]  x,x,1/4 [0,0,0]

6  f  ..2/m  1/2,0,0 [u,2u,0]  0,1/2,0 [2u,u,0]  1/2,1/2,0 [u,u,0]
     1/2,0,1/2 [u,2u,0]  0,1/2,1/2 [2u,u,0]  1/2,1/2,1/2 [u,u,0]

4  e  3.m  0,0,z [0,0,0]  0,0,z+1/2 [0,0,0]  0,0,z+1/2 [0,0,0]  0,0,z [0,0,0]

4  d  3.2  1/3,2,3/0 [0,0,0]  2/3,1/3,1/2 [0,0,0]  2/3,1/3,0 [0,0,0]  1/3,2/3,1/2 [0,0,0]

4  c  ..e  1/3,2,3,1/4 [0,0,w]  2/3,1/3,3/4 [0,0,w]  2/3,1/3,3/4 [0,0,w]  1/3,2/3,3/4 [0,0,w]

2  b  3.m  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]

2  a  62m  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p6mm1'  a* = a   b* = b
Along [1,0,0]  p2a-2mm  a* = c/2  b* = (a + 2b)/2
Along [2,1,0]  p2mg1'  a* = c   b* = b/2
Origin at 0,0,z  Origin at x,0,1/4  Origin at x,x/2,0
Origin at center (31m1') at 3c2/m1'

Asymmetric unit

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ≤ x ≤ 2/3;</td>
<td>0 ≤ y ≤ 1/2;</td>
<td>0 ≤ z ≤ 1/4;</td>
</tr>
<tr>
<td>x &lt; (1+y)/2;</td>
<td>y &lt; min (1-x,x)</td>
<td></td>
</tr>
</tbody>
</table>

Vertices

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>2/3,1/3,0</td>
</tr>
<tr>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
<td>2/3,1/3,1/4</td>
</tr>
<tr>
<td>1/2,1/2,0</td>
<td>1/2,1/2,1/4</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

For 1 + set

(1) 1
(1 | 0,0,0)

(2) 3+ 0,0,z
(3z | 0,0,0)

(3) 3- 0,0,z
(3z-1 | 0,0,0)

(4) 2 (0,0,1/2) 0,0,z
(2z | 0,0,1/2)

(5) 6- (0,0,1/2) 0,0,z
(6z-1 | 0,0,1/2)

(6) 6+ (0,0,1/2) 0,0,z
(6z | 0,0,1/2)

(7) 2 x,x,1/4
(2xy | 0,0,1/2)

(8) 2 x,0,1/4
(2z | 0,0,1/2)

(9) 2 0,y,1/4
(2y | 0,0,1/2)

(10) 2 x,x,0
(2z | 0,0,0)

(11) 2 x,2x,0
(2z | 0,0,0)

(12) 2 2x,x,0
(2z | 0,0,0)
(13) $\overline{1}$ 0,0,0
   $\langle \overline{1} \mid 0,0,0 \rangle$

(14) $\overline{3}'$ 0,0,z; 0,0,0
   $\langle \overline{3}' \mid 0,0,0 \rangle$

(15) $\overline{3}'$ 0,0,z; 0,0,0
   $\langle \overline{3}'_z \mid 0,0,0 \rangle$

(16) $m$ x,y,1/4
   $\langle m \mid 0,0,1/2 \rangle$

(17) $\bar{6}'$ 0,0,z; 0,0,1/4
   $\langle \bar{6}'_z \mid 0,0,1/2 \rangle$

(18) $\bar{6}'$ 0,0,z; 0,0,1/4
   $\langle \bar{6}'_z \mid 0,0,1/2 \rangle$

(19) $c$ (0,0,1/2) x,x,z
    $\langle m_y \mid 0,0,1/2 \rangle$

(20) $c$ (0,0,1/2) x,2x,z
    $\langle m_y \mid 0,0,1/2 \rangle$

(21) $c$ (0,0,1/2) 2x,x,z
    $\langle m_y \mid 0,0,1/2 \rangle$

(22) $m$ x,x,z
    $\langle m \mid 0,0,0 \rangle$

(23) $m$ x,0,z
    $\langle m \mid 0,0,0 \rangle$

(24) $m$ 0,y,z
    $\langle m \mid 0,0,0 \rangle$

For $1'$ + set

(1) $1'$
   $\langle 1 \mid 0,0,0 \rangle$

(1') $1'$
   $\langle 1' \mid 0,0,0 \rangle$

(2) $3''$ 0,0,z
   $\langle 3''_z \mid 0,0,0 \rangle$

(3) $3'$ 0,0,z
   $\langle 3' \mid 0,0,0 \rangle$

(4) $2'$ (0,0,1/2) 0,0,z
   $\langle 2' \mid 0,0,1/2 \rangle$

(5) $6'$ (0,0,1/2) 0,0,z
   $\langle 6' \mid 0,0,1/2 \rangle$

(6) $6'$ (0,0,1/2) 0,0,z
   $\langle 6' \mid 0,0,1/2 \rangle$

(7) $2'$ x,x,1/4
   $\langle 2' \mid 0,0,1/2 \rangle$

(8) $2'$ x,0,1/4
   $\langle 2' \mid 0,0,1/2 \rangle$

(9) $2'$ 0,y,1/4
   $\langle 2' \mid 0,0,1/2 \rangle$

(10) $2'$ x,x,0
    $\langle 2' \mid 0,0,0 \rangle$

(11) $2'$ x,2x,0
    $\langle 2' \mid 0,0,0 \rangle$

(12) $2'$ 2x,x,0
    $\langle 2' \mid 0,0,0 \rangle$

(13) $\bar{1}'$ 0,0,0
    $\langle \overline{1}' \mid 0,0,0 \rangle$

(14) $\overline{3}'$ 0,0,z; 0,0,0
    $\langle \overline{3}'_z \mid 0,0,0 \rangle$

(15) $\overline{3}'$ 0,0,z; 0,0,0
    $\langle \overline{3}'_z \mid 0,0,0 \rangle$

(16) $m'$ x,y,1/4
    $\langle m' \mid 0,0,1/2 \rangle$

(17) $\bar{6}'$ (0,0,1/2) 0,0,1/4
    $\langle \bar{6}' \mid 0,0,1/2 \rangle$

(18) $\bar{6}'$ (0,0,1/2) 0,0,1/4
    $\langle \bar{6}' \mid 0,0,1/2 \rangle$

(19) $c'$ (0,0,1/2) x,x,z
    $\langle m_y \mid 0,0,1/2 \rangle$

(20) $c'$ (0,0,1/2) x,2x,z
    $\langle m_y \mid 0,0,1/2 \rangle$

(21) $c'$ (0,0,1/2) 2x,x,z
    $\langle m_y \mid 0,0,1/2 \rangle$

(22) $m'$ x,x,z
    $\langle m' \mid 0,0,0 \rangle$

(23) $m'$ x,0,z
    $\langle m' \mid 0,0,0 \rangle$

(24) $m'$ 0,y,z
    $\langle m' \mid 0,0,0 \rangle$

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

\[
\begin{array}{ccc}
1 & + & 1' + \\
\hline
24 & l & 11' \\
(1) x,y,z [0,0,0] & (2) \bar{y},x-y,z [0,0,0] & (3) \bar{x}+y,x,z [0,0,0] \\
(4) \bar{x},y,z+1/2 [0,0,0] & (5) y,\bar{x}+y,z+1/2 [0,0,0] & (6) x-y,x,z+1/2 [0,0,0] \\
(7) y,x,z+1/2 [0,0,0] & (8) x-y,\bar{y},z+1/2 [0,0,0] & (9) \bar{x},x+y,z+1/2 [0,0,0] \\
(10) y,x,z [0,0,0] & (11) \bar{x}+y,y,z [0,0,0] & (12) x-x,y,\bar{z} [0,0,0] \\
\end{array}
\]
Symmetry of Special Projections

Along [0,0,1] p6mm1'
\[
a^* = a \quad b^* = b
\]
Origin at 0,0,z

Along [1,0,0] p2mm1'
\[
a^* = c/2 \quad b^* = (a + 2b)/2
\]
Origin at x,0,0

Along [2,1,0] p2mg1'
\[
a^* = c \quad b^* = b/2
\]
Origin at x,x/2,0
**Origin** at center (3‘1m) at 3‘c2/m

**Asymmetric unit**

<table>
<thead>
<tr>
<th>0 ≤ x ≤ 2/3;</th>
<th>0 ≤ y ≤ 1/2;</th>
<th>0 ≤ z ≤ 1/4;</th>
<th>x ≤ (1+y)/2;</th>
<th>y ≤ min (1-x,x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 0, 0</td>
<td>1/2, 0, 0</td>
<td>2/3, 1/3, 0</td>
<td>1/2, 1/2, 0</td>
<td></td>
</tr>
<tr>
<td>0, 0, 1/4</td>
<td>1/2, 0, 1/4</td>
<td>2/3, 1/3, 1/4</td>
<td>1/2, 1/2, 1/4</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry Operations**

1. 1
   (1 | 0, 0, 0)

2. 3‘ 0, 0, z
   (3z | 0, 0, 0)

3. 3‘ 0, 0, z
   (3z | 0, 0, 0)

4. 2 (0, 0, 1/2) 0, 0, z
   (2z | 0, 0, 1/2)

5. 6‘ (0, 0, 1/2) 0, 0, z
   (6z | 0, 0, 1/2)

6. 6‘ (0, 0, 1/2) 0, 0, z
   (6z | 0, 0, 1/2)

7. 2‘ x, x, 1/4
   (2xy | 0, 0, 1/2)‘

8. 2‘ x, 0, 1/4
   (2z | 0, 0, 1/2)‘

9. 2‘ 0, y, 1/4
   (2y | 0, 0, 1/2)‘

10. 2‘ x, x, 0
    (2x | 0, 0, 0)‘

11. 2‘ x, 2x, 0
    (2y | 0, 0, 0)‘

12. 2‘ 2x, x, 0
    (2z | 0, 0, 0)‘
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 l 1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z [v,u-w] (3) x+y,x,z [u-v,u-w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w] (5) y,x+y,z+1/2 [v,u+w] (6) x-y,x+z+1/2 [u-v,u-w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w] (8) x-y,y,z+1/2 [u+v,v,w] (9) x,x+y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) x,y,z [v,u,w] (11) x+y,y,z [u-v,v,w] (12) x,x-y,z+1/2 [u+u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(13) x,y,z [u,v,w] (14) y,x+y,z [v,u+v,w] (15) x,y,x,z [u-u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(16) x,y,z+1/2 [u,v,w] (17) y,x-y,z+1/2 [v,u-v,w] (18) x+y,x,z+1/2 [u+v,u+w]</td>
</tr>
<tr>
<td></td>
<td>(19) y,x,z+1/2 [v,u,w] (20) x+y,y,z+1/2 [u+v,v,w] (21) x,x-y,z+1/2 [u+u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(22) y,x,z [v,u,w] (23) x,y,z [u+v,v,w] (24) x,x+z [u-u+v,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 k ..m</td>
<td>x,0,z [u,2u,0] 0,x,z [2u,0,0] x,x,z [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,0,z+1/2 [u,2u,0] 0,x,z+1/2 [2u,0,0] x,x,z+1/2 [u,u,0]</td>
</tr>
<tr>
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<td>0,x,z+1/2 [2u,0,0] x,0,z+1/2 [u,2u,0] x,x,z+1/2 [u,u,0]</td>
</tr>
<tr>
<td></td>
<td>0,x,z [2u,0,0] 0,x,z [u,2u,0] x,x,z [u,u,0]</td>
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<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 j m'..</td>
<td>x,y,1/4 [u,v,0] y,x-y,1/4 [v,u-v,0] x+y,x,1/4 [u+v,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,3/4 [u,v,0] y,x+y,3/4 [v,u+v,0] x,y,x,3/4 [u-v,u,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,1/4 [v,u,0] x+y,x,1/4 [u+v,v,0] x+x+y,1/4 [u,u-v,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,3/4 [v,u,0] x+y,y,3/4 [u+v,v,0] x+y,x,3/4 [u-v,v,0]</td>
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<tr>
<td>12</td>
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<td>d</td>
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<tr>
<td>4</td>
<td>c</td>
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<tr>
<td>2</td>
<td>b</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
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</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm</th>
<th>Along [1,0,0]</th>
<th>p\text{*}2mm</th>
<th>Along [2,1,0]</th>
<th>p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a b* = b</td>
<td>a* = c/2 b* = (a + 2b)/2</td>
<td>a* = c b* = b/2</td>
<td>a* = c b* = b/2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at center (3'1m) at 3'c2'/m

**Asymmetric unit**

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad x < \frac{(1+y)}{2}; \quad y < \min(1-x,x)\]

**Vertices**

- \(0,0,0\)
- \(0,0,\frac{1}{4}\)
- \(1/2,0,0\)
- \(1/2,0,\frac{1}{4}\)
- \(2/3,1/3,0\)
- \(2/3,1/3,1/4\)
- \(1/2,1/2,0\)
- \(1/2,1/2,1/4\)

**Symmetry Operations**

1. \(1\)
2. \(3^+ \cdot 0,0,z\)
3. \(3^- \cdot 0,0,z\)
4. \(2' (0,0,1/2) \cdot 0,0,z\)
5. \(6^- \cdot (0,0,1/2) \cdot 0,0,z\)
6. \(6^+ \cdot (0,0,1/2) \cdot 0,0,z\)
7. \(2 \cdot x,x,1/4\)
8. \(2 \cdot x,0,1/4\)
9. \(2 \cdot 0,y,1/4\)
10. \(2' \cdot x,x,0\)
11. \(2' \cdot x,2x,0\)
12. \(2' \cdot 2x,x,0\)

193.4.1488 - 1 - 3276
Continued

193.4.1488

P6₃/mcm

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).</td>
<td>24 l 1 (1) x,y,z [u,v,w]</td>
<td>(2) y,x-y,z [v,u-v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
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<tr>
<td></td>
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<td>(4) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
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<td>(6) x+y,x,z+1/2 [u+v,u,w]</td>
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<tr>
<td></td>
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<td>(7) y,x,z+1/2 [v,u,w]</td>
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<td>(9) x,x+y,z+1/2 [u,u+v,w]</td>
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<td>(10) y,x,z [v,u,w]</td>
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<td>(12) x,y+z [u+v,u,w]</td>
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<td>(13) x,y,z [u,v,w]</td>
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<td>(15) x+y,x,z [u+v,u,w]</td>
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<td>(16) x,y,z+1/2 [u,v,w]</td>
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<td>(18) x+y,x,z+1/2 [u+v,u,w]</td>
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<td>(19) y,x,z+1/2 [v,u,w]</td>
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<td>(21) x,x+y,z+1/2 [u+v,u,w]</td>
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<td></td>
<td>(22) y,x,z [v,u,w]</td>
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<tr>
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<td></td>
<td>(24) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>12 k ..m x,0,z [u,2u,0]</td>
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<td>x,0,z+1/2 [u,2u,0]</td>
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<td>0,x,z+1/2 [2u,u,0]</td>
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<td>0,x,z [2u,u,0]</td>
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<td>x,0,z+1/2 [u,u,0]</td>
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<td></td>
<td>12 j m.. x,y,1/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>y,x+1/4 [0,0,w]</td>
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<td>y,y+1/4 [0,0,w]</td>
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<td>y,x+3/4 [0,0,w]</td>
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<tr>
<td></td>
<td></td>
<td>x+y,x+3/4 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>193.4.1488 - 2 - 3277</td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Operation</th>
<th>Symmetry</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p6mm1'</td>
<td>Origin at 0,0,z</td>
</tr>
</tbody>
</table>
| Along [1,0,0] | p2mm | $a^* = a$  
$\mathbf{b}^* = \mathbf{b}$  
Origin at x,0,0 |
| Along [2,1,0] | p2mg1' | $a^* = \mathbf{c}/2$  
$\mathbf{b}^* = (\mathbf{a}+2\mathbf{b})/2$  
Origin at x,x/2,0 |
Origin at center (3'1m') at 3'c2/m'

Asymmetric unit:

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad x \leq \frac{1+y}{2}; \quad y \leq \min (1-x, x) \]

Vertices:

- \( 0,0,0 \)
- \( 1/2,0,0 \)
- \( 2/3,1/3,0 \)
- \( 1/2,1/2,0 \)
- \( 0,0,1/4 \)
- \( 1/2,0,1/4 \)
- \( 2/3,1/3,1/4 \)
- \( 1/2,1/2,1/4 \)

Symmetry Operations:

1. \( 1 \)
2. \( 3^* \quad 0,0,0 \) \( z \) \( 3^* \quad 0,0,0 \)
3. \( 3^* \quad 0,0,0 \) \( z \) \( 3^* \quad 0,0,0 \)
4. \( 2' \quad 0,0,1/2 \) \( 0,0,z \) \( 2' \quad 0,0,1/2 \)
5. \( 6' \quad (0,0,1/2) \) \( 0,0,z \) \( 6' \quad (0,0,1/2) \)
6. \( 6' \quad (0,0,1/2) \) \( 0,0,z \) \( 6' \quad (0,0,1/2) \)
7. \( 2' \quad x,x,1/4 \) \( 2' \quad x,x,1/4 \) \( 2' \quad x,x,1/4 \)
8. \( 2' \quad x,0,1/4 \) \( 2' \quad x,0,1/4 \) \( 2' \quad x,0,1/4 \)
9. \( 2' \quad 0,y,1/4 \) \( 2' \quad 0,y,1/4 \) \( 2' \quad 0,y,1/4 \)
10. \( 2 \quad x,x,0 \) \( 2 \quad x,x,0 \) \( 2 \quad x,x,0 \)
11. \( 2 \quad x,2x,0 \) \( 2 \quad x,2x,0 \) \( 2 \quad x,2x,0 \)
12. \( 2 \quad 2x,x,0 \) \( 2 \quad 2x,x,0 \) \( 2 \quad 2x,x,0 \)
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 l 1</td>
<td>x,y,z [u,v,w]</td>
<td>(u+v,u,w)</td>
</tr>
<tr>
<td>24 l 1</td>
<td>x,y,z [u,v,w]</td>
<td>(u+v,u,w)</td>
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<td>24 l 1</td>
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<td>(u+v,u,w)</td>
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| Coordinates
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<th></th>
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<tr>
<td>1,2,3</td>
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<tr>
<td>1,2,3</td>
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</tbody>
</table>

| 12 k m'       | x,0,z [u,0,w] | (u,v,w) |
| 12 k m'       | x,0,z [u,0,w] | (u,v,w) |
| 12 k m'       | x,0,z [u,0,w] | (u,v,w) |
| 12 k m'       | x,0,z [u,0,w] | (u,v,w) |
| 12 k m'       | x,0,z [u,0,w] | (u,v,w) |

| 12 j m      | x,y,1/4 [0,0,w] | (0,0,u) |
| 12 j m      | x,y,1/4 [0,0,w] | (0,0,u) |
| 12 j m      | x,y,1/4 [0,0,w] | (0,0,u) |
| 12 j m      | x,y,1/4 [0,0,w] | (0,0,u) |
| 12 j m      | x,y,1/4 [0,0,w] | (0,0,u) |
Continued

<table>
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<tr>
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<th>h</th>
<th>g</th>
<th>f</th>
<th>e</th>
<th>d</th>
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</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm1'</th>
<th>Along [1,0,0]</th>
<th>p2m2m'm'</th>
<th>Along [2,1,0]</th>
<th>p2mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a )</td>
<td>( b^* = b )</td>
<td>( a^* = a ) ( b^* = b )</td>
<td>( a^* = c ) ( b^* = b/2 )</td>
<td>( a^* = c ) ( b^* = b/2 )</td>
<td>( a^* = c ) ( b^* = b/2 )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,0</td>
<td>Origin at x,x/2,0</td>
<td>Origin at x,x/2,0</td>
</tr>
</tbody>
</table>
**Origin** at center (31m) at 3c'2/m

**Asymmetric unit**

\[0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad x < \frac{(1+y)}{2}; \quad y \leq \min (1-x, x)\]

**Vertices**

- \(0,0,0\)
- \(1/2,0,0\)
- \(2/3,1/3,0\)
- \(1/2,1/2,0\)
- \(0,0,1/4\)
- \(1/2,0,1/4\)
- \(2/3,1/3,1/4\)
- \(1/2,1/2,1/4\)

**Symmetry Operations**

1. \(1\)
2. \(3^+ (0,0,0)\)
3. \(3^- (0,0,0)\)
4. \(2' (0,0,1/2) 0,0,z\)
5. \(6' (0,0,1/2) 0,0,z\)
6. \(6'' (0,0,1/2) 0,0,z\)
7. \(2' x,x,1/4\)
8. \(2' x,0,1/4\)
9. \(2' 0,y,1/4\)
10. \(2 x,x,0\)
11. \(2 x,2x,0\)
12. \(2 2x,x,0\)

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Continued

(13) $\overline{1}$ 0,0,0
    (1/1 0,0,0)

(14) $\overline{3}^\prime$ 0,0,z; 0,0,0
    (3) 0,0,0

(15) $\overline{3}^\prime$ 0,0,z; 0,0,0
    (3)$^1_2$ 0,0,0

(16) m$' \times,y,1/4$
    (m$('_y) 0,0,1/2')$

(17) $\overline{6}^\prime$ 0,0,z; 0,0,1/4
    (6)$^1_2$ 0,0,1/2')

(18) $\overline{6}^\prime$ 0,0,z; 0,0,1/4
    (6)$^3_2$ 0,0,1/2')

(19) c$'$ (0,0,1/2) x,x,z
    (m$('_x) 0,0,1/2')$

(20) c$'$ (0,0,1/2) x,2x,z
    (m$('_x) 0,0,1/2')$

(21) c$'$ (0,0,1/2) 2x,x,z
    (m$('_y) 0,0,1/2')$

(22) m x,x,z
    (m$('_x) 0,0,0)$

(23) m x,0,z
    (m$('_z) 0,0,0)$

(24) m 0,y,z
    (m$('_z) 0,0,0)$

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>1,1</td>
<td>(1) x,y,z [u,v,w] (2) $\overline{y},x$-y,z [$\overline{v}$,u-v,w] (3) $\overline{x}$+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) $\overline{x}$,y,z+1/2 [u,v,w] (5) $\overline{y}$,x+y,z+1/2 [$\overline{v}$,u-v,w] (6) x-y,x,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(7) y,x,z+1/2 [$v$,u,w] (8) x-y,$\overline{y}$,z+1/2 [$\overline{u}$+v,v,w] (9) $\overline{x}$,x+y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
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<td></td>
<td>(10) y,x,z [$v$,u,w] (11) $\overline{x}$+y,y,z [$\overline{u}$+v,v,w] (12) x-x,z [$u-u,v,w$]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(13) $\overline{x}$,y,z [$u,v,w$] (14) y,$\overline{x}$+y,z [$\overline{v}$,u-v,w] (15) x-y,x,z [$u+v,u,w$]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(16) x,y,z+1/2 [u,v,w] (17) $\overline{y}$,x-y,z+1/2 [$\overline{v}$,u-v,w] (18) $\overline{x}$+y,x,z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(19) y,$\overline{x}$,z+1/2 [$\overline{v}$,u,w] (20) $\overline{x}$+y,y,z+1/2 [$\overline{u}$+v,v,w] (21) x-x,z+1/2 [u,u-v,w]</td>
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<tr>
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<td>(22) x,x,z [$v$,u,w] (23) x-y,$\overline{y}$,z [$\overline{u}$+v,v,w] (24) $\overline{x}$,x+y,z [$u-u,v,w$]</td>
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</tbody>
</table>

| 12           | k ..m   | x,0,z [u,2u,0] 0,x,z [2u,0,0] $\overline{x}$,x,z [u,u,0] |
|              |          | x,0,z+1/2 [u,2u,0] 0,x,z+1/2 [2u,0,0] x,x,z+1/2 [u,u,0] |
|              |          | 0,x,z+1/2 [2u,0,0] x,0,z+1/2 [u,2u,0] $\overline{x}$,x,z+1/2 [u,u,0] |
|              |          | 0,x,z [2u,0,0] $\overline{x}$,0,z [u,2u,0] x,x,z [u,u,0] |

<p>| 12           | j m$'$. | x,y,1/4 [u,v,0] $\overline{y}$,x-y,1/4 [$\overline{v}$,u-v,0] $\overline{x}$+y,x,1/4 [$\overline{u}$+v,u,0] |
|              |          | $\overline{x}$,$\overline{y}$,3/4 [u,v,0] y,x+y,3/4 [$\overline{v}$,u-v,0] x-y,x,3/4 [$\overline{u}$+v,u,0] |
|              |          | y,x,1/4 [$\overline{v}$,u,0] x-y,$\overline{y}$,1/4 [$\overline{u}$+v,v,0] $\overline{x}$+y,x,1/4 [u,u-v,0] |
|              |          | y,$\overline{x}$,3/4 [$\overline{v}$,u,0] $\overline{x}$+y,y,3/4 [$\overline{u}$+v,v,0] x,x-y,3/4 [u,u-v,0] |</p>
<table>
<thead>
<tr>
<th>i</th>
<th>2/m'</th>
<th>x,2x,0 [u,2u,0]</th>
<th>2x,x,0 [2u, u,0]</th>
<th>x,x,0 [u, u,0]</th>
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<td>2x,x,1/2 [2u, u,0]</td>
<td>x,x,1/2 [u, u,0]</td>
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<td>2x,x,0 [2u, u,0]</td>
<td>x,x,0 [u, u,0]</td>
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<td>x,2x,1/2 [u,2u,0]</td>
<td>2x,x,1/2 [2u, u,0]</td>
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<table>
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<th>3..</th>
<th>1/3,2/3,z [0,0,w]</th>
<th>2/3,1/3,z+1/2 [0,0,w]</th>
<th>2/3,1/3,z [0,0,w]</th>
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<tbody>
<tr>
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<td>2/3,1/3,z+1/2 [0,0,w]</td>
<td>1/3,2/3,z+1/2 [0,0,w]</td>
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<table>
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<tr>
<th>g</th>
<th>m'2'm</th>
<th>x,0,1/4 [u,2u,0]</th>
<th>0,x,1/4 [2u, u,0]</th>
<th>x,x,1/4 [u, u,0]</th>
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</thead>
<tbody>
<tr>
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<td>x,0,3/4 [u,2u,0]</td>
<td>0,x,3/4 [2u, u,0]</td>
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<table>
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<th>f</th>
<th>.2/m</th>
<th>1/2,0,0 [u,2u,0]</th>
<th>0,1/2,0 [2u, u,0]</th>
<th>1/2,1/2,0 [u, u,0]</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1/2,0,1/2 [u,2u,0]</td>
<td>0,1/2,1/2 [2u, u,0]</td>
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</tr>
</tbody>
</table>

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<tr>
<th>e</th>
<th>3.m</th>
<th>0,0,z [0,0,0]</th>
<th>0,0,z+1/2 [0,0,0]</th>
<th>0,0,z [0,0,0]</th>
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<td>0,0,z+1/2 [0,0,0]</td>
<td>0,0,z [0,0,0]</td>
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<th>d</th>
<th>3.2</th>
<th>1/3,2/3,0 [0,0,0]</th>
<th>2/3,1/3,1/2 [0,0,0]</th>
<th>2/3,1/3,0 [0,0,0]</th>
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<td>2/3,1/3,1/2 [0,0,0]</td>
<td>2/3,1/3,0 [0,0,0]</td>
<td>1/3,2/3,1/2 [0,0,0]</td>
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</table>

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<th>c</th>
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<th>2/3,1/3,3/4 [0,0,0]</th>
<th>2/3,1/3,1/4 [0,0,0]</th>
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<td>2/3,1/3,1/4 [0,0,0]</td>
<td>1/3,2/3,3/4 [0,0,0]</td>
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</table>

| b  | 3.m  | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |

| a  | 6'2'm | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] | 0,0,3/4 [0,0,0] |

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along</th>
<th>p6'm'm</th>
<th>Along</th>
<th>p2'm'm'</th>
<th>Along</th>
<th>p2mg1'</th>
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</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (a + 2b)/2</td>
<td>b* = c/2</td>
<td>a* = c</td>
<td>b* = b/2</td>
</tr>
</tbody>
</table>

Origin at 0,0,0, Origin at 0,0,0, Origin at x,0,0, Origin at x,x/2,0,
Origin at center (31m') at 3c2/m'

Asymmetric unit

$$0 \leq x \leq 2/3; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad x \leq (1+y)/2; \quad y \leq \min(1-x,x)$$

Vertices

\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 2/3,1/3,0 & \quad 1/2,1/2,0 \\
0,0,1/4 & \quad 1/2,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/2,1/2,1/4
\end{align*}

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3 \quad 0,0,z \\
(4) & \quad 2' \quad (0,0,1/2) \quad 0,0,z \\
(5) & \quad 6' \quad (0,0,1/2) \quad 0,0,z \\
(6) & \quad 6' \quad (0,0,1/2) \quad 0,0,z \\
(7) & \quad 2 \quad x,x,1/4 \\
(8) & \quad 2 \quad x,0,1/4 \\
(9) & \quad 2 \quad 0,y,1/4 \\
(10) & \quad 2' \quad x,x,0 \\
(11) & \quad 2' \quad x,0,1/2 \\
(12) & \quad 2' \quad 2x,x,0
\end{align*}
Continued 193.7.1491 P6$_3'/m'$cm'

(13) $1$ 0,0,0  
(14) $3'$ 0,0,0; 0,0,0  
(15) $3'$ 0,0,0; 0,0,0  

(16) m' x,y,1/4  
(m$_0$| 0,0,1/2)'  
(17) $6'$ 0,0,1/4  
(6'$_z$| 0,0,1/2)'  
(18) $6'$ 0,0,1/4  
(6'$_z$| 0,0,1/2)'  

(19) c (0,0,1/2)  
(m$_y$| 0,0,1/2)  
(20) c (0,0,1/2)  
(m$_y$| 0,0,1/2)  
(21) c (0,0,1/2)  
(22) m' x,x,z  
(m$_3$| 0,0,0)'  
(23) m' x,0,z  
(m$_2$| 0,0,0)'  
(24) m' 0,y,z  
(m$_1$| 0,0,0)'  

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
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<td>24 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
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<tr>
<td></td>
<td>(2) y,x,y,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u+w]</td>
</tr>
<tr>
<td></td>
<td>(4) x',y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+y,x,z+1/2 [u+v,u+w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x-y,y,z+1/2 [u-v,v,w]</td>
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<tr>
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<td>(9) x,x+y,z+1/2 [u+u+v,w]</td>
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<tr>
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<td>(10) y,x,z [v,u,w]</td>
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<td>(11) x+y,y,z [u-v,v,w]</td>
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<td>(12) x,x+y,z [u+u+v,w]</td>
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<td>(13) x,y,z [u,v,w]</td>
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<td>(14) y,x+y,z [v,u+w]</td>
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<td></td>
<td>(15) x+y,x,z [u+v,u,w]</td>
</tr>
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<td>(16) x,y,z+1/2 [u,v,w]</td>
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<td>(17) y,x-y,z+1/2 [v,u-v,w]</td>
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<tr>
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<td>(18) x+y,x,z+1/2 [u+v,u+w]</td>
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<td>(19) y,x,z+1/2 [v,u,w]</td>
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<td>(20) x+y,y,z+1/2 [u-v,v+w]</td>
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<tr>
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<td>(21) x,x-y,z+1/2 [u+u+v,w]</td>
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<td>(22) y,x,z [v,u,w]</td>
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<td>(23) x-y,y,z [u-v,v+w]</td>
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<td>(24) x,x+y,z [u+u+v,w]</td>
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<td>x,0,z+1/2 [0,u,w]</td>
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<tr>
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<td>x,x,z [u,u,w]</td>
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<tr>
<td>12 j m'.</td>
<td>x,y,1/4 [u,v,0]</td>
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<tr>
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<td>y,x-y,1/4 [v,u-v,0]</td>
</tr>
<tr>
<td></td>
<td>x+y,x,1/4 [u+v,u,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,3/4 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>y,x+y,3/4 [v,u-v,0]</td>
</tr>
<tr>
<td></td>
<td>x+y,x,3/4 [u+v,u,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,1/4 [v,u,0]</td>
</tr>
<tr>
<td></td>
<td>x-y,y,1/4 [u-v,v,0]</td>
</tr>
<tr>
<td></td>
<td>x+x+y,1/4 [u+u+v,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,3/4 [v,u,0]</td>
</tr>
<tr>
<td></td>
<td>x+y,y,3/4 [u-v,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,x-y,3/4 [u+u+v,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along \([0,0,1]\) \(p6'\overline{m}m'\) \(a^* = a\) \(b^* = b\)  
Origin at 0,0,z

Along \([1,0,0]\) \(p_{2a}2m'm'\) \(a^* = c/2\) \(b^* = (a + 2b)/2\)  
Origin at x,0,1/4

Along \([2,1,0]\) \(p2'm'g\) \(a^* = c\) \(b^* = b/2\)  
Origin at x,x/2,0
Origin at center (3 1m') at 3c'2'/m'

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad x \leq (1+y)/2; \quad y \leq \min (1-x, x) \]

Vertices

\[
\begin{align*}
0,0,0 & : 1/2,0,0 & : 2/3,1/3,0 & : 1/2,1/2,0 \\
0,0,1/4 & : 1/2,0,1/4 & : 2/3,1/3,1/4 & : 1/2,1/2,1/4
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & : 1 \\
(1) & : (1|0,0,0) \\
(4) & : 2 \ (0,0,1/2) \ 0,0,z \\
(2z) & : 0,0,1/2 \\
(7) & : 2' \ x,x,1/4 \\
(2x) & : 0,0,1/2' \\
(10) & : 2' \ x,x,0 \\
(2z) & : 0,0,0') \\
(2) & : 3^* \ 0,0,z \\
(3) & : (3_z) \ 0,0,0 \\
(5) & : 6^* \ (0,0,1/2) \ 0,0,z \\
(6) & : (6_z) \ 0,0,1/2 \\
(8) & : 2' \ x,0,1/4 \\
(2x) & : 0,0,1/2' \\
(11) & : 2' \ x,2x,0 \\
(2z) & : 0,0,0') \\
(12) & : 2' \ 2x,x,0 \\
(2z) & : 0,0,0')
\end{align*}
\]
Continued

<table>
<thead>
<tr>
<th>Position</th>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 l 1</td>
<td>1,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>(13) 0,0,0</td>
<td>0,0,0</td>
<td>(14) 0,0,0,0</td>
</tr>
<tr>
<td>(16) m x,y/1</td>
<td>0,0,0,0,0,0</td>
<td>(17) 0,0,0,0,0,0</td>
</tr>
<tr>
<td>(19) c' (0,0,1/2) x,x,z</td>
<td>0,0,0,0,0,0</td>
<td>(20) c' (0,0,1/2) x,x,z</td>
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<tr>
<td>(22) m' x,x,z</td>
<td>0,0,0,0,0,0</td>
<td>(23) m' x,x,z</td>
</tr>
</tbody>
</table>

Generators selected (1); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 k m' x,0,z [u,0,w]</td>
<td>0,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,x,z [0,0,0]</td>
</tr>
<tr>
<td>12 j m.. x,y,1/4 [0,0,0]</td>
<td>x+y,x,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>x,x+y,1/4 [0,0,0]</td>
</tr>
<tr>
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<td>x,x+y,1/4 [0,0,0]</td>
</tr>
<tr>
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<td>x,x+y,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Generators selected (1); t(0,1,0); t(0,0,1); (2); (4); (7); (13).
## Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Number</th>
<th>Type</th>
<th>Expansion</th>
<th>Axes</th>
<th>Result</th>
<th>Axes</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 i</td>
<td>.2'</td>
<td>x,2x,0 [u,0,w]</td>
<td>2x,x,0 [0,u,w]</td>
<td>x,x,0 [u,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,1/2 [u,0,w]</td>
<td>2x,x,1/2 [0,u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,0 [u,0,w]</td>
<td>2x,x,0 [0,u,w]</td>
<td>x,x,0 [u,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,2x,1/2 [u,0,w]</td>
<td>2x,x,1/2 [0,u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 h</td>
<td>3..</td>
<td>1/3,2/3,3z [0,0,w]</td>
<td>2/3,1/3,3z+1/2 [0,0,w]</td>
<td>1/3,2/3,3z [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2/3,1/3,3z [0,0,w]</td>
<td>1/3,2/3,3z+1/2 [0,0,w]</td>
<td>2/3,1/3,3z [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6 g</td>
<td>m2'm'</td>
<td>x,0,1/4 [0,0,w]</td>
<td>0,x,1/4 [0,0,w]</td>
<td>x,x,1/4 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,0,3/4 [0,0,w]</td>
<td>0,x,3/4 [0,0,w]</td>
<td>x,x,3/4 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6 f</td>
<td>.2'm'</td>
<td>1/2,0,0 [u,0,w]</td>
<td>0,1/2,0 [u,u,w]</td>
<td>1/2,1/2,0 [u,u,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,0,1/2 [u,0,w]</td>
<td>0,1/2,1/2 [u,u,w]</td>
<td>1/2,1/2,1/2 [u,u,w]</td>
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<td></td>
</tr>
<tr>
<td>4 e</td>
<td>3.m'</td>
<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>4 d</td>
<td>3.2'</td>
<td>1/3,2/3,0 [0,0,w]</td>
<td>2/3,1/3,1/2 [0,0,w]</td>
<td>1/3,2/3,1/2 [0,0,w]</td>
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<td></td>
</tr>
<tr>
<td>4 c</td>
<td>6..</td>
<td>1/3,2/3,1/4 [0,0,w]</td>
<td>2/3,1/3,3/4 [0,0,w]</td>
<td>1/3,2/3,3/4 [0,0,w]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 b</td>
<td>3.m'</td>
<td>0,0,0 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 a</td>
<td>62'm'</td>
<td>0,0,1/4 [0,0,w]</td>
<td>0,0,3/4 [0,0,w]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p6mm
  - Origin at 0,0,z
  - Projection: p6mm
  - a* = a  b* = b

- **Along [1,0,0]**: p2mm
  - Origin at x,0,0
  - Projection: p2mm
  - a* = c/2  b* = (a + 2b)/2

- **Along [2,1,0]**: p2mg
  - Origin at x,x/2,0
  - Projection: p2mg
  - a* = c  b* = b/2
Origin at center (31m') at 3c'2/m'

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad x \leq \frac{(1+y)}{2}; \quad y \leq \min(1-x,x) \]

Vertices

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0</td>
<td>0,0</td>
<td>0,0</td>
</tr>
<tr>
<td>0,0</td>
<td>1/2,0,0</td>
<td></td>
</tr>
<tr>
<td>0,0,1/4</td>
<td>1/2,0,1/4</td>
<td></td>
</tr>
<tr>
<td>2/3,1/3,0</td>
<td>2/3,1/3,1/4</td>
<td></td>
</tr>
<tr>
<td>1/2,1/2,0</td>
<td>1/2,1/2,1/4</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

(1) 1  
(1 | 0,0,0) 

(2) 3' 0,0,z  
(3' | 0,0,0) 

(3) 3' 0,0,z  
(3' | 0,0,0) 

(4) 2 (0,0,1/2) 0,0,z  
(2 | 0,0,1/2) 

(5) 6' (0,0,1/2) 0,0,z  
(6' | 0,0,1/2) 

(6) 6' (0,0,1/2) 0,0,z  
(6' | 0,0,1/2) 

(7) 2 x,x,1/4  
(2 | 0,0,1/2) 

(8) 2 x,0,1/4  
(2 | 0,0,1/2) 

(9) 2 0,y,1/4  
(2 | 0,0,1/2) 

(10) 2 x,x,0  
(2 | 0,0,0) 

(11) 2 x,2x,0  
(2 | 0,0,0) 

(12) 2 2x,x,0  
(2 | 0,0,0)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>24 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(13) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(14) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(15) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(16) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(17) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(18) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(19) x,y,z [u,v,w]</td>
</tr>
<tr>
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<td>(20) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(21) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(22) x,y,z [u,v,w]</td>
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<td></td>
<td>(23) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(24) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

| 12 k m'      | x,0,z [u,0,w] |
|              | x,0,z [u,0,w] |
|              | 0,x,z [0,u,w] |
|              | 0,x,z [0,u,w] |
|              | 0,x,z [0,u,w] |
|              | 0,x,z [0,u,w] |
|              | 0,x,z [0,u,w] |
|              | 0,x,z [0,u,w] |
|              | 0,x,z [0,u,w] |

| 12 j m'      | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
|              | x,y,1/4 [u,v,0] |
| 12 | i   | .2 | x,2x,0 [u,2u,0] | 2x, x,0 [2u, u,0] | x, x,0 [u, u,0] |
| 8  | h 3 | 1/3,2/3,z [0,0,w] | 2/3,1/3,z+1/2 [0,0,w] | 1/3,2/3,z [0,0,w] |
| 6  | g m'2m' | x,0,1/4 [u,0,0] | 0,x,1/4 [0,u,0] | x, x,1/4 [u, u,0] |
| 6  | f .2/m' | 1/2,0,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 4  | e 3.m' | 0,0,z [0,0,w] | 0,0,z+1/2 [0,0,w] | 0,0,z [0,0,w] |
| 4  | d 3.2 | 1/3,2/3,0 [0,0,0] | 2/3,1/3,1/2 [0,0,0] | 1/3,2/3,1/2 [0,0,0] |
| 4  | c 6'.. | 1/3,2/3,1/4 [0,0,0] | 2/3,1/3,3/4 [0,0,0] | 1/3,2/3,3/4 [0,0,0] |
| 2  | b 3'.m' | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] |
| 2  | a 6'2m' | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p6m'm'  
Along [1,0,0] p2m'm'  
Along [2,1,0] p2m'g'  

a* = a  b* = b  
Origin at 0,0,z  

a* = c/2  b* = (a + 2b)/2  
Origin at x,0,0  

a* = c  b* = b/2  
Origin at x,x/2,0
Origin at center (3m1) at 32/mc

Asymmetric unit

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; 0 ≤ z ≤ 1/4; x ≤ 2y; y ≤ min(1-x,2x)

Vertices

0,0,0 2/3,1/3,0 1/3,2/3,0
0,0,1/4 2/3,1/3,1/4 1/3,2/3,1/4

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 3+ 0,0,z
(3) 3- 0,0,z
(3_0,0,0)

(3) 3- 0,0,z
(3_0,0,0)

(4) 2 (0,0,1/2) 0,0,z
(2, 0,0,1/2)

(5) 6' (0,0,1/2) 0,0,z
(6_0,0,1/2)

(6) 6' (0,0,1/2) 0,0,z
(6_0,0,1/2)

(7) 2 x,x,0
(2, x,0,0)

(8) 2 x,0,0
(2, x,0,0)

(9) 2 0,y,0
(2, y,0,0)

(10) 2 x,x,1/4
(2, x,0,1/2)

(11) 2 x,2x,1/4
(2, x,0,1/2)

(12) 2 2x,x,1/4
(2, x,0,1/2)
### Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
</table>

### Coordinates

<table>
<thead>
<tr>
<th>24</th>
<th>l</th>
<th>1</th>
<th>x,y,z [u,v,w]</th>
<th>y,x-y,z [v,u-v,w]</th>
<th>x+y,x,z [u+v,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>k</td>
<td>.m.</td>
<td>x,2x,z [u,0,0]</td>
<td>2x,x,z [0,u,0]</td>
<td>x,x,z [u,u,0]</td>
</tr>
<tr>
<td>12</td>
<td>j</td>
<td>m..</td>
<td>x,y,1/4 [0,0,w]</td>
<td>y,x-y,1/4 [0,0,w]</td>
<td>x+y,x,1/4 [0,0,w]</td>
</tr>
</tbody>
</table>

The table above lists the coordinates and multiplicity of positions in the unit cell, along with the site symmetry for each position.
Continued 194.1.1494 P6$_3$/mmc

12  i  2.  x,0,0 [u,0,0]  0.x,0 [0,u,0]  \( \vec{x},0,0 [u,\vec{u},0] \)
   \( \vec{x},0,1/2 [\vec{u},0,0] \)  0.x,1/2 [0,\vec{u},0]  \( \vec{x},x,1/2 [u,\vec{u},0] \)
   \( \vec{x},0,0 [u,0,0] \)  0.x,0 [0,u,0]  \( \vec{x},x,0 [\vec{u},\vec{u},0] \)
   \( x,0,1/2 [u,0,0] \)  0.x,1/2 [0,\vec{u},0]  \( \vec{x},\vec{x},1/2 [u,u,0] \)

6  h  mm2  x,2x,1/4 [0,0,0]  2x,x,1/4 [0,0,0]  \( \vec{x},\vec{x},1/4 [0,0,0] \)
   \( \vec{x},2x,3/4 [0,0,0] \)  2x,x,3/4 [0,0,0]  \( \vec{x},\vec{x},3/4 [0,0,0] \)

6  g  .2/m.  1/2,0,0 [u,0,0]  0,1/2,0 [0,u,0]  \( 1/2,1/2,0 [\vec{u},\vec{u},0] \)
   \( 1/2,0,1/2 [\vec{u},0,0] \)  0,1/2,1/2 [0,\vec{u},0]  \( 1/2,1/2,1/2 [u,u,0] \)

4  f  3m.  1/3,2/3,z [0,0,0]  2/3,1/3,z+1/2 [0,0,0]  \( 2/3,1/3,z [0,0,0] \)
   \( 2/3,1/3,z+1/2 [0,0,0] \)  \( 1/3,2/3,z+1/2 [0,0,0] \)

4  e  3m.  0,0,z [0,0,0]  0,0,z+1/2 [0,0,0]  \( 0,0,z [0,0,0] \)
   \( 0,0,z+1/2 [0,0,0] \)

2  d  \( \bar{6}m2 \)  1/3,2/3,3/4 [0,0,0]  2/3,1/3,1/4 [0,0,0]

2  c  \( \bar{6}m2 \)  1/3,2/3,1/4 [0,0,0]  2/3,1/3,3/4 [0,0,0]

2  b  \( \bar{6}m2 \)  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]

2  a  \( 3m. \)  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6mm1'</th>
<th>Along [1,0,0]</th>
<th>p2mg1'</th>
<th>Along [2,1,0]</th>
<th>p$_{2a}$2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{a}^* = \mathbf{a} )</td>
<td>( \mathbf{b}^* = \mathbf{b} )</td>
<td>( \mathbf{a}^* = \mathbf{c} )</td>
<td>( \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b})/2 )</td>
<td>( \mathbf{a}^* = \mathbf{c}/2 )</td>
<td>( \mathbf{b}^* = \mathbf{b}/2 )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,0,0</td>
<td>Origin at x,x/2,1/4</td>
<td>Origin at x,x/2,1/4</td>
<td>Origin at x,x/2,1/4</td>
<td>Origin at x,x/2,1/4</td>
</tr>
</tbody>
</table>

194.1.1494 - 3 - 3296
Origin at center (3m11') at 32/mc1'

Asymmetric unit

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; 0 ≤ z ≤ 1/4; x < 2y; y ≤ min(1-x,2x)

Vertices

0,0,0 2/3,1/3,0 1/3,2/3,0
0,0,1/4 2/3,1/3,1/4 1/3,2/3,1/4

Symmetry Operations

For 1 + set

1
(1 | 0,0,0)

(1) 1

(2) 3⁰ 0,0,z
(3z | 0,0,0)

(3) 3⁻ 0,0,z
(3z⁻¹ | 0,0,0)

(4) 2 (0,0,1/2) 0,0,z
(2z | 0,0,1/2)

(5) 6⁻ (0,0,1/2) 0,0,z
(6z⁻¹ | 0,0,1/2)

(6) 6⁺ (0,0,1/2) 0,0,z
(6z | 0,0,1/2)

(7) 2 x,x,0
(2xy | 0,0,0)

(8) 2 x,0,0
(2z | 0,0,0)

(9) 2 0,y,0
(2y | 0,0,0)

(10) 2 x,x,1/4
(2z | 0,0,1/2)

(11) 2 x,2x,1/4
(2z | 0,0,1/2)

(12) 2 2x,x,1/4
(2z | 0,0,1/2)
Continued

Generators selected

For 1' + set

Generators selected

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

1 + 1' +
(13) $x, y, z + [0,0,0]$  
(14) $y, x + y, z + [0,0,0]$  
(15) $x-y, x, z + [0,0,0]$  
(16) $x, y, z + 1/2 + [0,0,0]$  
(17) $y, x, y, z + 1/2 + [0,0,0]$  
(18) $x+y, x, z + 1/2 + [0,0,0]$  
(19) $y, x, z + [0,0,0]$  
(20) $x+y, y, z + [0,0,0]$  
(21) $x, y, z + 1/2 + [0,0,0]$  
(22) $x, y, z + 1/2 + [0,0,0]$  
(23) $x-y, y, z + [0,0,0]$  
(24) $x, x+y, z + 1/2 + [0,0,0]$  

12 k .m.1' 
$x, 2x, z + [0,0,0]$  
$x, 2x, z + 1/2 + [0,0,0]$  
$2x, x, z + [0,0,0]$  
$2x, x, z + 1/2 + [0,0,0]$  

12 j m..1' 
$x, 1/4 + [0,0,0]$  
$y, x-y, 1/4 + [0,0,0]$  
$y, x, 3/4 + [0,0,0]$  
$y, x, y, 3/4 + [0,0,0]$  

12 i .21' 
$x, 0, 0 + [0,0,0]$  
$x, 0, 1/2 + [0,0,0]$  
$x, 0, 0 + [0,0,0]$  
$x, 0, 1/2 + [0,0,0]$  

6 h mm21' 
$x, 2x, 1/4 + [0,0,0]$  
$x, 2x, 3/4 + [0,0,0]$  

6 g .2/m.1' 
$1/2, 0, 0 + [0,0,0]$  
$1/2, 0, 1/2 + [0,0,0]$  

4 f 3m.1' 
$1/3, 2/3, z + [0,0,0]$  
$2/3, 1/3, z + [0,0,0]$  

4 e 3m.1' 
$0, 0, z + [0,0,0]$  
$0, 0, z + 1/2 + [0,0,0]$  

2 d 6m21' 
$1/3, 2/3, 3/4 + [0,0,0]$  

2 c 6m21' 
$1/3, 2/3, 1/4 + [0,0,0]$  

2 b 6m21' 
$0, 0, 1/4 + [0,0,0]$  

2 a 3m.1' 
$0, 0, 0 + [0,0,0]$  
$0, 0, 1/2 + [0,0,0]$
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry Group</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p6mm1'</td>
<td>$a^* = a$  \quad b^* = b$</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at $0,0,z$</td>
</tr>
<tr>
<td>Along [1,0,0]</td>
<td>p2mg1'</td>
<td>$a^* = c$  \quad b^* = (a + 2b)/2</td>
</tr>
<tr>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at $x,0,0$</td>
</tr>
<tr>
<td>Along [2,1,0]</td>
<td>p2mm1'</td>
<td>$a^* = c/2$  \quad b^* = b/2</td>
</tr>
<tr>
<td>Origin at x,x/2,0</td>
<td></td>
<td>Origin at $x,x/2,0$</td>
</tr>
</tbody>
</table>
Origin at center (3'm1) at 3'2'/mc

Asymmetric unit

0 ≤ x ≤ 2/3; 0 ≤ y ≤ 2/3; 0 ≤ z ≤ 1/4; x ≤ 2y; y ≤ min(1-x, 2x)

Vertices

0,0,0 2/3,1/3,0 1/3,2/3,0
0,0,1/4 2/3,1/3,1/4 1/3,2/3,1/4

Symmetry Operations

(1) 1
(1 | 0,0,0)

(2) 3' 0,0,z
(3'z | 0,0,0)

(3) 3' -1 0,0,z
(3'z -1 | 0,0,0)

(4) 2 (0,0,1/2) 0,0,z
(2z | 0,0,1/2)

(5) 6' (0,0,1/2) 0,0,z
(6'z -1 | 0,0,1/2)

(6) 6' -1 (0,0,1/2) 0,0,z
(6z | 0,0,1/2)

(7) 2' x,x,0
(2xy | 0,0,0)'

(8) 2' x,0,0
(2z | 0,0,0)'

(9) 2' x, y,0
(2y | 0,0,0)'

(10) 2' x,x,1/4
(2xy | 0,0,1/2)'

(11) 2' x,x,1/4
(2z | 0,0,1/2)'

(12) 2' 2x,x,1/4
(2z | 0,0,1/2)'

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Continued

<table>
<thead>
<tr>
<th>13</th>
<th>m’ 0,0,0</th>
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</thead>
<tbody>
<tr>
<td>(1)</td>
<td>1,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>14</th>
<th>3’</th>
<th>0,0,0; 0,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2)</td>
<td>3</td>
<td>0,0,0; 0,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>15</th>
<th>3’</th>
<th>0,0,0; 0,0,0</th>
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</thead>
<tbody>
<tr>
<td>(3)</td>
<td>3</td>
<td>0,0,0; 0,0,0</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>16</th>
<th>m' x,y,1/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>m</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>17</th>
<th>6’</th>
<th>0,0,0; 0,0,1/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2)</td>
<td>6</td>
<td>0,0,0; 0,0,1/4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>18</th>
<th>6’</th>
<th>0,0,0; 0,0,1/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3)</td>
<td>6</td>
<td>0,0,0; 0,0,1/4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>19</th>
<th>m x,z</th>
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</thead>
<tbody>
<tr>
<td>(1)</td>
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</table>

<table>
<thead>
<tr>
<th>20</th>
<th>m x,2x,z</th>
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<tbody>
<tr>
<td>(2)</td>
<td>m</td>
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</table>

<table>
<thead>
<tr>
<th>21</th>
<th>m 2x,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3)</td>
<td>m</td>
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</table>

<table>
<thead>
<tr>
<th>22</th>
<th>c (0,0,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>c</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>23</th>
<th>c (0,0,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2)</td>
<td>c</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>24</th>
<th>c (0,0,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3)</td>
<td>c</td>
</tr>
</tbody>
</table>

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) y,x,y,z [v,u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) y,x+y,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x+y,x,z+1/2 [u,v+w]</td>
</tr>
<tr>
<td></td>
<td>(7) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y,z [u+v,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x+y,z [u,u+w]</td>
</tr>
<tr>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x+y,x,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x+y,x,z+1/2 [u,v+w]</td>
</tr>
<tr>
<td></td>
<td>(13) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(14) x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(15) y,x,z [u,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(16) x,y,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(17) x+y,x,z+1/2 [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(18) x+y,x,z+1/2 [u+v,u+w]</td>
</tr>
<tr>
<td></td>
<td>(19) y,x,z [v,u,w]</td>
</tr>
<tr>
<td></td>
<td>(20) x+y,z [v,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(21) x+y,z [u,u+v,w]</td>
</tr>
<tr>
<td></td>
<td>(22) x,y,z+1/2 [v,u+w]</td>
</tr>
<tr>
<td></td>
<td>(23) x+y,z+1/2 [u+v,v+w]</td>
</tr>
</tbody>
</table>

| 12 k m'       | x,2x,z [u,0,0] |
|              | 2x,x,z [0,u,0] |
|              | x,x,z [u,u,0] |
|              | x,2x,z+1/2 [u,0,0] |
|              | 2x,x,z+1/2 [0,u,0] |
|              | 2x,x,z [u,0,0] |
|              | x,2x,z [u,0,0] |
|              | x,x,z [u,u,0] |
|              | 2x,x,z+1/2 [0,u,0] |
|              | x,2x,z+1/2 [u,0,0] |
|              | x,x,z+1/2 [u,u,0] |

| 12 j m'       | x,y,1/4 [u,v,0] |
|              | y,x,y,1/4 [v,u-v,0] |
|              | x+y,x,1/4 [u+v,u,0] |
|              | x,y,3/4 [u,v,0] |
|              | y,x,3/4 [v,u,0] |
|              | y,x,3/4 [u,v,0] |
|              | y,x,3/4 [v,u,0] |
|              | y,x,3/4 [u,v,0] |
|              | x+y,x,1/4 [u+v,u,0] |
|              | x,x-y,1/4 [u,u+v,0] |
Continued 194.3.1496 P6₃/m'm'c

12  i .2'.  x,0,0 [u,2u,w]  0,x,0 [2u,−u,w]  x,x,0 [u,u,w]  
   −x,0,1/2 [u,2u,w]  0,x,1/2 [2u,u,w]  x,x,1/2 [u,u,w]  
   −xx,0,0 [u,2u,−w]  0,xx,0 [2u,u,−w]  xx,x,0 [u,−u,w]  
   −x,0,1/2 [u,2u,−w]  0,x,1/2 [2u,−u,−w]  xx,x,1/2 [u,−u,−w]  
6  h m'm2'  x,2x,1/4 [u,0,0]  2x,−x,1/4 [0,u,0]  x,−x,1/4 [u,u,0]  
   −x,2x,3/4 [u,0,0]  2x,−x,3/4 [0,−u,0]  x,−x,3/4 [u,−u,0]  
6  g .2'm.  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  
   1/2,0,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  
4  f 3m.  1/3,2/3,z [0,0,0]  2/3,1/3,z+1/2 [0,0,0]  2/3,1/3,z [0,0,0]  1/3,2/3,z+1/2 [0,0,0]  
4  e 3m.  0,0,0 [0,0,0]  0,0,z [0,0,0]  0,0,z [0,0,0]  0,0,z+1/2 [0,0,0]  
2  d 6'm2'  1/3,2/3,3/4 [0,0,0]  2/3,1/3,1/4 [0,0,0]  2/3,1/3,1/4 [0,0,0]  
2  c 6'm2'  1/3,2/3,1/4 [0,0,0]  2/3,1/3,3/4 [0,0,0]  2/3,1/3,3/4 [0,0,0]  
2  b 6'm2'  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]  0,0,3/4 [0,0,0]  
2  a 3'm.  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1]  p6mm  Along [1,0,0]  p2mg1'  Along [2,1,0]  p2a,2mm  
\(a^* = a \quad b^* = b\)  \(a^* = c \quad b^* = (a + 2b)/2\)  \(a^* = c/2 \quad b^* = b/2\)  
Origin at 0,0,z  Origin at x,0,0  Origin at x,x/2,0  

194.3.1496 - 3 - 3303
Origin at center (3\textsuperscript{1}m'1) at 3\textsuperscript{1}2/m'c

Asymmetric unit

\[ 0 \leq x \leq \frac{2}{3}; \quad 0 \leq y \leq \frac{2}{3}; \quad 0 \leq z \leq \frac{1}{4}; \quad x < 2y; \quad y \leq \min(1-x, 2x) \]

Vertices

- \(0, 0, 0\)
- \(2/3, 1/3, 0\)
- \(1/3, 2/3, 0\)
- \(0, 0, 1/4\)
- \(2/3, 1/3, 1/4\)
- \(1/3, 2/3, 1/4\)

Symmetry Operations

1. \(1\)
2. \(3^* \cdot 0,0,z\)
3. \(3^* \cdot 0,0,0\)
4. \(2' \cdot (0,0,1/2) \cdot 0,0,z\)
5. \(6' \cdot (0,0,1/2) \cdot 0,0,z\)
6. \(6' \cdot (0,0,1/2) \cdot 0,0,z\)
7. \(2 \cdot x,x,0\)
8. \(2 \cdot x,0,0\)
9. \(2 \cdot 0,y,0\)
10. \(2' \cdot x,x,1/4\)
11. \(2' \cdot x,2x,1/4\)
12. \(2' \cdot 2x,x,1/4\)
Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

Continued

\[ (13) \overset{t}{0,0,0} \quad (14) \overset{3}{0,0,z; 0,0,0} \quad (15) \overset{3}{0,0,z; 0,0,0} \]
\[ (16) \overset{m}{x,y,1/4} \quad (17) \overset{6}{0,0,z; 0,0,1/4} \quad (18) \overset{6}{0,0,z; 0,0,1/4} \]
\[ (19) \overset{m'}{x,x,z} \quad (20) \overset{m'}{x,2x,z} \quad (21) \overset{m'}{2x,x,z} \]
\[ (22) \overset{c}{0,0,1/2} x,x,z \quad (23) \overset{c}{0,0,1/2} x,0,z \quad (24) \overset{c}{0,0,1/2} 0,y,z \]

24 l 1 \( (1) x,y,z \ [u,v,w] \quad (2) \bar{y},x-y,z \ [\bar{v},u-v,w] \quad (3) x+y,x,z \ [\bar{u}+v,\bar{u},w] \)
\( (4) \bar{x},y,z+1/2 \ [u,v,w] \quad (5) y,x+y,z+1/2 \ [v,u-v,w] \quad (6) x-y,x,z+1/2 \ [u-v,u,w] \)
\( (7) y,x,z \ [v,u,w] \quad (8) x-y,x-z \ [u-v,v,w] \quad (9) x+y,x,z \ [\bar{u}+v,\bar{u},w] \)
\( (10) \bar{y},x,z+1/2 \ [v,u,w] \quad (11) \bar{x}+y,z+1/2 \ [u-v,\bar{v},w] \quad (12) x-x-y,z+1/2 \ [\bar{u},\bar{u}+v,\bar{w}] \)
\( (13) \bar{x},y,z \ [u,v,\bar{w}] \quad (14) \bar{y},x+y,z \ [v,u+v,\bar{w}] \quad (15) y-x-y,z \ [\bar{u},u+v,\bar{w}] \)
\( (16) x,y,z+1/2 \ [\bar{v},\bar{u},w] \quad (17) \bar{y}-x,y,z+1/2 \ [v,u+v,\bar{w}] \quad (18) \bar{x}+y,x,z+1/2 \ [u-v,u,w] \)
\( (19) y,x,z \ [v,\bar{u},w] \quad (20) \bar{x}+y,y,z \ [u+v,v,w] \quad (21) x-x-y,z \ [u-u-v,\bar{w}] \)
\( (22) x,x,z+1/2 \ [\bar{v},\bar{u},w] \quad (23) x-y,x,z+1/2 \ [u-v,v,\bar{w}] \quad (24) x-x,y,z+1/2 \ [u-u-v,\bar{w}] \)

12 k \( .m'. \quad x,2x,z \ [u,2u,w] \quad 2x,x,z \ [2u,u,w] \quad x,x,z \ [u,\bar{u},w] \)
\( \bar{x},2x,z+1/2 \ [u,2u,w] \quad 2x,x,z+1/2 \ [2u,\bar{u},w] \quad \bar{x},x,z+1/2 \ [u,\bar{u},w] \)
\( 2x,x,z \ [2u,u,w] \quad \bar{x},2x,z \ [u,2u,w] \quad \bar{x},x,z \ [u,\bar{u},w] \)
\( 2x,x,z+1/2 \ [2u,u,w] \quad x,2x,z+1/2 \ [2u,\bar{u},w] \quad x,x,z+1/2 \ [u,\bar{u},w] \)

12 j \( m'. \quad x,y,1/4 \ [0,0,w] \quad \bar{y},x-y,1/4 \ [0,0,w] \quad x+y,x,1/4 \ [0,0,w] \)
\( \bar{x},y,3/4 \ [0,0,w] \quad y,x+y,3/4 \ [0,0,w] \quad x-y,x,3/4 \ [0,0,w] \)
\( y,x,3/4 \ [0,0,w] \quad x-y,y,3/4 \ [0,0,w] \quad \bar{x}+y,x,3/4 \ [0,0,\bar{w}] \)
\( y,x,1/4 \ [0,0,w] \quad x+y,y,1/4 \ [0,0,w] \quad x-x-y,1/4 \ [0,0,w] \)
12  i  .2.  x,0,0 [u,0,0]  0,x,0 [0,u,0]  x,x,0 [u,0,0]  
    \hspace{1cm}  x,0,1/2 [u,0,0]  0,x,1/2 [0,u,0]  x,x,1/2 [u,u,0]  
    \hspace{1cm}  x,0,0 [u,0,0]  0,x,0 [0,0,0]  x,x,0 [u,u,0]  
    \hspace{1cm}  x,0,1/2 [u,0,0]  0,x,1/2 [0,u,0]  x,x,1/2 [u,u,0]  
   
6  h  mm'2'  x,2x,1/4 [0,0,w]  2x,x,1/4 [0,0,w]  x,x,1/4 [0,0,w]  
    \hspace{1cm}  x,2x,3/4 [0,0,w]  2x,x,3/4 [0,0,w]  x,x,3/4 [0,0,w]  
   
6  g  .2/m'.  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  
    \hspace{1cm}  1/2,0,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  
   
4  f  3m'.  1/3,2/3,z [0,0,w]  2/3,1/3,z+1/2 [0,0,w]  2/3,1/3,z [0,0,w]  
    \hspace{1cm}  1/3,2/3,z+1/2 [0,0,w]  2/3,1/3,z+1/2 [0,0,w]  1/3,2/3,z+1/2 [0,0,w]  
   
4  e  3m'.  0,0,z [0,0,w]  0,0,z+1/2 [0,0,w]  0,0,z [0,0,w]  
    \hspace{1cm}  0,0,z+1/2 [0,0,w]  0,0,z+1/2 [0,0,w]  0,0,z+1/2 [0,0,w]  
   
2  d  \bar{6}m'2'  1/3,2/3,3/4 [0,0,w]  2/3,1/3,3/4 [0,0,w]  
    \hspace{1cm}  2/3,1/3,3/4 [0,0,w]  2/3,1/3,3/4 [0,0,w]  
   
2  c  \bar{6}m'2'  1/3,2/3,1/4 [0,0,w]  2/3,1/3,1/4 [0,0,w]  
    \hspace{1cm}  2/3,1/3,1/4 [0,0,w]  2/3,1/3,1/4 [0,0,w]  
   
2  b  \bar{6}m'2'  0,0,1/4 [0,0,w]  0,0,3/4 [0,0,w]  
    \hspace{1cm}  0,0,3/4 [0,0,w]  0,0,3/4 [0,0,w]  
   
2  a  3'm'.  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]  
    \hspace{1cm}  0,0,1/2 [0,0,0]  0,0,1/2 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1]  p6mm1'  
  a* = a  b* = b  
  Origin at 0,0,z  

Along [1,0,0]  p2mg  
  a* = c  b* = (a + 2b)/2  
  Origin at x,0,0  

Along [2,1,0]  p_{2a},2m'm'  
  a* = c/2  b* = b/2  
  Origin at x,x/2,0
**Origin** at center \((3'm1)\) at \(3'2'mc'\)

**Asymmetric unit**  
\[0 \leq x \leq 2/3\];  
\[0 \leq y \leq 2/3\];  
\[0 \leq z \leq 1/4\];  
\[x < 2y\];  
\[y \leq \min(1-x,2x)\]

**Vertices**  
\[0,0,0\]  
\[2/3,1/3,0\]  
\[1/3,2/3,0\]  
\[0,0,1/4\]  
\[2/3,1/3,1/4\]  
\[1/3,2/3,1/4\]

**Symmetry Operations**

1. \(1\)  
   \((1|0,0,0)\)

2. \(3^+\)  
   \((0,0,z)\)
   \((3_z|0,0,0)\)

3. \(3^-\)  
   \((0,0,z)\)
   \((3_z^{-1}|0,0,0)\)

4. \(2'\)  
   \((0,0,1/2)\)
   \((0,0,z)\)
   \((2_z|0,0,1/2)\)

5. \(6'\)  
   \((0,0,1/2)\)
   \((0,0,z)\)
   \((6_x^{-1}|0,0,1/2)\)

6. \(6''\)  
   \((0,0,1/2)\)
   \((0,0,z)\)
   \((6_z|0,0,1/2)\)

7. \(2'\)  
   \((x,x,0)\)
   \((2_{xy}|0,0,0)\)

8. \(2'\)  
   \((x,0,0)\)
   \((2_z|0,0,0)\)

9. \(2'\)  
   \((y,0,0)\)
   \((2_y|0,0,0)\)

10. \(2\)  
    \((x,1/4)\)
    \((2_z|0,0,1/2)\)

11. \(2\)  
    \((x,1/4)\)
    \((2_{xy}|0,0,0)\)

12. \(2\)  
    \((2x,1/4)\)
    \((2_z|0,0,1/2)\)
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
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<td>24</td>
<td>l 1</td>
</tr>
<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2)</td>
<td>y,x-y,z [u-v,v,w]</td>
</tr>
<tr>
<td>(3)</td>
<td>x+y,x,z [u+v,u,w]</td>
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<tr>
<td>(4)</td>
<td>x,y,z+1/2 [u,v,w]</td>
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<td>(5)</td>
<td>y,x+y,z+1/2 [v,u-w]</td>
</tr>
<tr>
<td>(6)</td>
<td>x+y,x,z+1/2 [u-v,v,w]</td>
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<tr>
<td>(7)</td>
<td>y,x,z [v,u,w]</td>
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<tr>
<td>(8)</td>
<td>x-y,x,y [u-v,w]</td>
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<tr>
<td>(9)</td>
<td>x,x+y,z [u-u,v,w]</td>
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<td>y,x,z+1/2 [v,u,w]</td>
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<td>x,y,z+1/2 [u,v,w]</td>
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<td>(17)</td>
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<td>x+y,x,z+1/2 [v+v+w]</td>
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<td>y,x,z [v,u,w]</td>
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<td>y,x,z+1/2 [v,u,w]</td>
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<tr>
<td>(23)</td>
<td>x-y,x,y+1/2 [u-v,w]</td>
</tr>
<tr>
<td>(24)</td>
<td>x,x+y,z+1/2 [u-u+v,w]</td>
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</table>

12

k .m.  
x,x+2, z [u,0,0]  
\(x, x+z+1/2 [u, 0, 0]\)  
2x,x [0,0,0]  
\(x, z+1/2 [u, 0, 0]\)  
\(x, z+1/2 [u, 0, 0]\)

12

j m..  
x,y,1/4 [0,0,w]  
\(y, x, y, 1/4 [0, 0, w]\)  
\(y, x, y, 1/4 [0, 0, w]\)  
\(x+y, x, y, 1/4 [0, 0, w]\)  
\(x+y, x, 1/4 [0, 0, w]\)
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>12</th>
<th>i</th>
<th>.2'</th>
<th>x,0,0 [u,2u,w]</th>
<th>0,x,0 [2u,u,w]</th>
<th>x,x,0 [u,u,w]</th>
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<tbody>
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<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x,0,0 [2u,2u,w]</td>
<td>0,x,0 [2u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
</tr>
</tbody>
</table>

| 6 | h | mm2 | x,2x,1/4 [0,0,0] | 2x,x,1/4 [0,0,0] | x,x,1/4 [0,0,0] |
|   |   |     | x,2x,3/4 [0,0,0] | 2x,x,3/4 [0,0,0] | x,x,3/4 [0,0,0] |

| 6 | g | .2'/m. | 1/2,0,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
|   |   |       | 1/2,0,1/2 [0,0,0] | 0,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

| 4 | f | 3m. | 1/3,2/3,z [0,0,0] | 2/3,1/3,z+1/2 [0,0,0] | 2/3,1/3,z [0,0,0] |
|   |   |     | 2/3,1/3,z+1/2 [0,0,0] | 2/3,1/3,z+1/2 [0,0,0] | 2/3,1/3,z+1/2 [0,0,0] |

| 4 | e | 3m. | 0,0,z [0,0,0] | 0,0,z+1/2 [0,0,0] | 0,0,z [0,0,0] |
|   |   |     | 0,0,z+1/2 [0,0,0] | 0,0,z+1/2 [0,0,0] | 0,0,z+1/2 [0,0,0] |

| 2 | d | 6m2 | 1/3,2/3,3/4 [0,0,0] | 2/3,1/3,1/4 [0,0,0] | 2/3,1/3,1/4 [0,0,0] |
|   |   |     | 2/3,1/3,3/4 [0,0,0] | 2/3,1/3,3/4 [0,0,0] | 2/3,1/3,3/4 [0,0,0] |

| 2 | c | 6m2 | 0,0,1/4 [0,0,0] | 0,0,3/4 [0,0,0] | 0,0,3/4 [0,0,0] |
|   |   |     | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |

| 2 | b | 3m. | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |
|   |   |     | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |

| 2 | a | 3'm. | 0,0,0 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |
|   |   |     | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |

### Symmetry Relations

- **a** = a, **b** = b
- **a** = c, **b** = (a + 2b)/2
- **a** = c/2, **b** = b/2
**Origin** at center \((3\,m\,1)\) at \(\overline{3}2/m'c\)

**Asymmetric unit**

\[
0 < x < \frac{2}{3}; \quad 0 < y < \frac{2}{3}; \quad 0 < z < \frac{1}{4}; \quad x < 2y; \quad y \leq \min(1-x,2x)
\]

**Vertices**

\[
\begin{align*}
0, 0, 0 & \quad 2/3, 1/3, 0 \quad 1/3, 2/3, 0 \\
0, 0, 1/4 & \quad 2/3, 1/3, 1/4 \quad 1/3, 2/3, 1/4
\end{align*}
\]

**Symmetry Operations**

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0, 0, 0 \\
(4) & \quad 2' \ (0, 0, 1/2) \ 0, 0, z \\
(2z & \quad 0, 0, 1/2)' \\
(7) & \quad 2' \ x, x, 0 \\
(2y & \quad 0, 0, 0)' \\
(10) & \quad 2 \ x, x, 1/4 \\
(2 & \quad 0, 0, 1/2)
\end{align*}
\]

\[
\begin{align*}
(2) & \quad 3^+ \ 0, 0, z \\
(3z & \quad 0, 0, 0) \\
(5) & \quad 6' \ (0, 0, 1/2) \ 0, 0, z \\
(6z & \quad 0, 0, 1/2)' \\
(8) & \quad 2' \ x, 0, 0 \\
(2z & \quad 0, 0, 0)' \\
(11) & \quad 2 \ x, 2x, 1/4 \\
(2z & \quad 0, 0, 1/2)
\end{align*}
\]

\[
\begin{align*}
(3) & \quad 3^- \ 0, 0, z \\
(3z & \quad 0, 0, 0) \\
(6) & \quad 6^+ \ (0, 0, 1/2) \ 0, 0, z \\
(6z & \quad 0, 0, 1/2)' \\
(9) & \quad 2' \ 0, y, 0 \\
(2y & \quad 0, 0, 0)' \\
(12) & \quad 2 \ 2x, x, 1/4 \\
(2z & \quad 0, 0, 1/2)
\end{align*}
\]
Continued

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Position</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>24</td>
<td>l 1</td>
<td>(1) x,y,z [u,v,w] (2) y,x-y,z [v-u,v,w] (3) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td></td>
<td></td>
<td>(7) y,x,z [v,u,w] (8) x-y,x,z [u+v,v,w] (9) x+y,x,z [u,u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(10) y,x,z+1/2 [v,u,w]</td>
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<tr>
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<td>(13) x,y,z [u,v,w] (14) y,x+y,z [v-u,v,w] (15) x+y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(16) x,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(19) y,x,z [v,u,w] (20) x+y,x,z [u+v,v,w] (21) x+y,x,z [u,u-v,v,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(22) y,x,z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>12</td>
<td>k m'</td>
<td>x,2x,z [u,2u,w]</td>
</tr>
<tr>
<td></td>
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<td>x,2x,z+1/2 [u,2u,w]</td>
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<td>2x,x,z [2u,u,w]</td>
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<tr>
<td>12</td>
<td>j m'</td>
<td>x,y,1/4 [u,v,0]</td>
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<td>x,y,3/4 [u,v,0]</td>
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<td>y,x,3/4 [v,u,0]</td>
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</table>
12 i .2'. x,0,0 [u,2u,w] 0,x,0 [2u, u,w] x,x,0 [u,u,w] 

x,0,1/2 [u,2u,w] 0,x,1/2 [2u, u,w] x,x,1/2 [u,u,w] 

x,0,0 [u,2u,w] 0,x,0 [2u, u,w] x,x,0 [u,u,w] 

x,0,1/2 [u,2u,w] 0,x,1/2 [2u, u,w] x,x,1/2 [u,u,w] 

6 h m'm'2 x,2x,1/4 [u,2u,0] 2x,x,1/4 [2u, u,0] x,x,1/4 [u,u,0] 

x,2x,3/4 [u,2u,0] 2x,x,3/4 [2u, u,0] x,x,3/4 [u,u,0] 

6 g .2'/m'. 1/2,0,0 [u,2u,w] 0,1/2,0 [2u, u,w] 1/2,1/2,0 [u,u,w] 

1/2,0,1/2 [u,2u,w] 0,1/2,1/2 [2u, u,w] 1/2,1/2,1/2 [u,u,w] 

4 f 3m'. 1/3,2/3,z [0,0,w] 2/3,1/3,z+1/2 [0,0,w] 2/3,1/3,2z [0,0,w] 1/3,2/3,z+1/2 [0,0,w] 

4 e 3m'. 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w] 0,0,z [0,0,w] 0,0,z+1/2 [0,0,w] 

2 d 6'm'2 1/3,2/3,3/4 [0,0,0] 2/3,1/3,1/4 [0,0,0] 

2 c 6'm'2 1/3,2/3,1/4 [0,0,0] 2/3,1/3,3/4 [0,0,0] 

2 b 6'm'2 0,0,1/4 [0,0,0] 0,0,3/4 [0,0,0] 

2 a 3m'. 0,0,0 [0,0,w] 0,0,1/2 [0,0,w] 

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p6m'm'</th>
<th>Along [1,0,0]</th>
<th>p2'm'g</th>
<th>Along [2,1,0]</th>
<th>p2a.2m'm'</th>
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<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = c</td>
<td>a* = (a + 2b)/2</td>
<td>a* = c/2</td>
<td>b* = b/2</td>
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<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,0,0</td>
<td></td>
<td>Origin at x,x/2,1/4</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (3m1) at 32/mc'

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x < 2y; \quad y \leq \min(1-x,2x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2/3,0 \\
0,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/3,2/3,1/4
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 & \quad (1*0,0,0) \\
(2) & \quad 3' \quad 0,0,z & \quad (3_z*0,0,0) \\
(3) & \quad 3' \quad 0,0,z & \quad (3_z^-*0,0,0) \\
(4) & \quad 2' \quad (0,0,1/2) \quad 0,0,z & \quad (2_z*0,0,1/2) \\
(5) & \quad 6' \quad (0,0,1/2) \quad 0,0,z & \quad (6_z^-*0,0,1/2) \\
(6) & \quad 6' \quad (0,0,1/2) \quad 0,0,z & \quad (6_z*0,0,1/2) \\
(7) & \quad 2 \quad x,x,0 & \quad (2_x*0,0,0) \\
(8) & \quad 2 \quad x,0,0 & \quad (2_y*0,0,0) \\
(9) & \quad 2 \quad 0,y,0 & \quad (2_y*0,0,0) \\
(10) & \quad 2' \quad x,x,1/4 & \quad (2_z*0,0,1/2) \\
(11) & \quad 2' \quad x,2x,1/4 & \quad (2_z*0,0,1/2) \\
(12) & \quad 2' \quad 2x,x,1/4 & \quad (2_z*0,0,1/2) \\
\end{align*}
\]
(13) $\vec{1}$ 0,0,0
(14) $\vec{3}'$ 0,0,0; 0,0,0
(15) $\vec{3}'$ 0,0,0; 0,0,0

(16) $m' x,y,1/4$
$m' x,y,1/4$

(17) $6' - 0,0,1/4$
$6' - 0,0,1/4$

(19) $m x,x,z$
$m x,x,z$

(22) $c' (0,0,1/2) x,x,z$
$c' (0,0,1/2) x,x,z$

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>24</td>
<td>l</td>
<td>1</td>
</tr>
<tr>
<td>12</td>
<td>k</td>
<td>.m.</td>
</tr>
<tr>
<td>12</td>
<td>j</td>
<td>m'.</td>
</tr>
</tbody>
</table>

Coordinates

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<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>(2)</td>
<td>y,x-y,z [v,u-v,w]</td>
<td>x+y,x,z [u+v,u,w]</td>
<td>(3)</td>
</tr>
<tr>
<td>(5)</td>
<td>y,x+y,z+1/2 [v,u-v,w]</td>
<td>(6)</td>
<td>x-y,x,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td>(8)</td>
<td>x-y,y,z [u-v,v,w]</td>
<td>(9)</td>
<td>x,x+y,z [u,u+v,w]</td>
</tr>
<tr>
<td>(11)</td>
<td>x+y,y,z+1/2 [v,u-v,w]</td>
<td>(12)</td>
<td>x-x-y,z+1/2 [u,u-v,w]</td>
</tr>
<tr>
<td>(14)</td>
<td>y,x+y,z [v,u-v,w]</td>
<td>(15)</td>
<td>x-y,x,z [u+v,u,w]</td>
</tr>
<tr>
<td>(17)</td>
<td>y,x-y,z+1/2 [v,u-v,w]</td>
<td>(18)</td>
<td>x-y,x-z+1/2 [u+v,u,w]</td>
</tr>
<tr>
<td>(20)</td>
<td>x+y,y,z [u-v,v,w]</td>
<td>(21)</td>
<td>x-x-y,z [u,u+v,w]</td>
</tr>
<tr>
<td>(23)</td>
<td>x-y,y,z+1/2 [v,u-v,w]</td>
<td>(24)</td>
<td>x-y,x,z+1/2 [u,u+v,w]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

**Along [0,0,1] p6'mm'**

\( a^* = a \) \hspace{1cm} \( b^* = b \)  
Origin at 0,0,z

**Along [1,0,0] p2mg1'**

\( a^* = c \) \hspace{1cm} \( b^*(a + 2b)/2 \)  
Origin at x,0,0

**Along [2,1,0] p2'mm'**

\( a^* = b/2 \) \hspace{1cm} \( b^* = c/2 \)  
Origin at x,x/2,0
Origin at center (3m'1) at 32'/m'c'

Asymmetric unit

\[ 0 \leq x \leq 2/3; \quad 0 \leq y \leq 2/3; \quad 0 \leq z \leq 1/4; \quad x < 2y; \quad y \leq \min(1-x,2x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 2/3,1/3,0 & \quad 1/3,2,3,0 \\
0,0,1/4 & \quad 2/3,1/3,1/4 & \quad 1/3,2,3,1/4
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^* \quad 0,0,z \\
(3) & \quad 3^* \quad 0,0,z \\
(4) & \quad 2 (0,0,1/2) \quad 0,0,z \\
(5) & \quad 6^- (0,0,1/2) \quad 0,0,z \\
(6) & \quad 6^- (0,0,1/2) \quad 0,0,z \\
(7) & \quad 2' \quad x,x,0 \\
(8) & \quad 2' \quad x,0,0 \\
(9) & \quad 2' \quad y,0,0 \\
(10) & \quad 2' \quad x,x,1/4 \\
(11) & \quad 2' \quad x,2x,1/4 \\
(12) & \quad 2' \quad 2x,x,1/4 \quad (2,0,0,0)' \quad (2,0,0,0)' \quad (2,0,0,0)'
\end{align*}
\]
Continued

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<td>$\overline{1}$</td>
<td>0,0,0</td>
<td>$\overline{1}$</td>
<td>0,0,0</td>
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</tr>
<tr>
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<td>$\overline{3}$</td>
<td>0,0,z; 0,0,0</td>
<td>$\overline{3}$</td>
<td>0,0,z; 0,0,0</td>
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</tr>
<tr>
<td>15</td>
<td>$\overline{3}$</td>
<td>0,0,z; 0,0,0</td>
<td>$\overline{3}$</td>
<td>0,0,0</td>
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<tr>
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<td>x,y,1/4</td>
<td>m'</td>
<td>0,0,1/2</td>
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</tr>
<tr>
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<td>0,0,z; 0,0,1/4</td>
<td>$\overline{6}$</td>
<td>0,0,1/2</td>
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<tr>
<td>18</td>
<td>m'</td>
<td>x,y,1/4</td>
<td>m'</td>
<td>0,0,0'</td>
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<td>19</td>
<td>(m')</td>
<td>x,x,z</td>
<td>(m')</td>
<td>0,0,0'</td>
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<td>0,0,1/2)</td>
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<td>22</td>
<td>x'</td>
<td>(0,0,1/2)</td>
<td>x,y,1/4</td>
<td>(23)</td>
<td>(0,0,1/2)</td>
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Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>24 l 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(4) x,y,z+1/2 [u,v,w]</td>
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</tr>
<tr>
<td>(7) y,x,z [u,v,w]</td>
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<td>(10) y,x,z+1/2 [v,u,w]</td>
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<td>(13) x,y,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(16) x,y,z+1/2 [u,v,w]</td>
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<tr>
<td>(19) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(22) y,x,z+1/2 [v,u,w]</td>
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</tr>
<tr>
<td>12 k m'</td>
<td>x,2x,z [u,2u,w]</td>
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<tr>
<td>x,2x,z+1/2 [u,2u,w]</td>
<td></td>
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<tr>
<td>2x,x,z [2u,u,w]</td>
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<td>2x,x,z+1/2 [2u,u,w]</td>
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<tr>
<td>12 j m'</td>
<td>x,y,1/4 [0,0,w]</td>
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<td>x,y,3/4 [0,0,w]</td>
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Continued

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<th>12</th>
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<th>.2'</th>
<th>x,0,0 [u,2u,w]</th>
<th>0,x,0 [2u,u,w]</th>
<th>x,x,0 [u,u,w]</th>
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</thead>
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<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
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<td></td>
<td></td>
<td>x,0,0 [u,2u,w]</td>
<td>0,x,0 [2u,u,w]</td>
<td>x,x,0 [u,u,w]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x,0,1/2 [u,2u,w]</td>
<td>0,x,1/2 [2u,u,w]</td>
<td>x,x,1/2 [u,u,w]</td>
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<table>
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<th>6</th>
<th>h</th>
<th>mm'2'</th>
<th>x,2x,1/4 [0,0,w]</th>
<th>2x,x,1/4 [0,0,w]</th>
<th>x,x,1/4 [0,0,w]</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
<td>x,2x,3/4 [0,0,w]</td>
<td>2x,x,3/4 [0,0,w]</td>
<td>x,x,3/4 [0,0,w]</td>
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<table>
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<tr>
<th>6</th>
<th>g</th>
<th>.2'/m'</th>
<th>1/2,0,0 [u,2u,w]</th>
<th>0,1/2,0 [2u,u,w]</th>
<th>1/2,1/2,0 [u,u,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,0,1/2 [u,2u,w]</td>
<td>0,1/2,1/2 [2u,u,w]</td>
<td>1/2,1/2,1/2 [u,u,w]</td>
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<table>
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<tr>
<th>4</th>
<th>f</th>
<th>3m'</th>
<th>1/3,2/3,z [0,0,w]</th>
<th>2/3,1/3,z+1/2 [0,0,w]</th>
<th>2/3,1/3,z [0,0,w]</th>
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<tbody>
<tr>
<td></td>
<td></td>
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<td>0,0,z [0,0,w]</td>
<td>0,0,z+1/2 [0,0,w]</td>
<td>0,0,z [0,0,w]</td>
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<table>
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<tr>
<th>2</th>
<th>d</th>
<th>6m'2'</th>
<th>1/3,2/3,3/4 [0,0,w]</th>
<th>2/3,1/3,1/4 [0,0,w]</th>
<th>2/3,1/3,1/4 [0,0,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/3,2/3,1/4 [0,0,w]</td>
<td>2/3,1/3,3/4 [0,0,w]</td>
<td>2/3,1/3,3/4 [0,0,w]</td>
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</table>

<table>
<thead>
<tr>
<th>2</th>
<th>b</th>
<th>6m'2'</th>
<th>0,0,1/4 [0,0,w]</th>
<th>0,0,3/4 [0,0,w]</th>
<th>0,0,3/4 [0,0,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
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<td>0,0,0 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
<td>0,0,1/2 [0,0,w]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p6mm1'  
**a**' = **a**  
**b**' = **b**  
Origin at 0,0,z

Along [1,0,0] p2'mg'  
**a**' = **c**  
**b**' = (**a** + 2**b**) / 2  
Origin at x,0,0

Along [2,1,0] p2'mm'  
**a**' = c/2  
**b**' = **b**/2  
Origin at x,x/2,0
Origin at center \((3 \text{m}^1)\) at \(3\overline{2}/m\text{c'}\)

Asymmetric unit:
- \(0 \leq x \leq 2/3;\)  \(0 \leq y \leq 2/3;\)  \(0 \leq z \leq 1/4;\)  \(x < 2y;\)  \(y \leq \min(1-x,2x)\)

Vertices:
- \(0,0,0\)
- \(2/3,1/3,0\)
- \(1/3,2/3,0\)
- \(0,0,1/4\)
- \(2/3,1/3,1/4\)
- \(1/3,2/3,1/4\)

Symmetry Operations:

1. \(1\)
2* \(0,0,z\)

2. \(3\) \(0,0,0\)

3. \(3\) \(0,0,z\)

4. \(2\)

5. \(6\)

6. \(6\)

7. \(2\)

8. \(2\)

9. \(2\)

10. \(2\)

11. \(2\)

12. \(2\)
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (4); (7); (13).

Positions

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<td>(19) y,x,z [v,u,w]</td>
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<tr>
<td></td>
<td>(22) y,x,z+1/2 [v,u,w]</td>
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<tr>
<td>12 k .m'</td>
<td>x,2x,z [u,2u,w]</td>
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<tr>
<td></td>
<td>x,2x,z+1/2 [u,2u,w]</td>
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<tr>
<td></td>
<td>2x,x,z [2u,u,w]</td>
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<td>x,2x,z+1/2 [2u,u,w]</td>
</tr>
<tr>
<td>12 j .m'</td>
<td>x,y,1/4 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>x,y,3/4 [u,v,0]</td>
</tr>
<tr>
<td></td>
<td>y,x,3/4 [v,u,0]</td>
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<tr>
<td></td>
<td>y,x,1/4 [v,u,0]</td>
</tr>
</tbody>
</table>
12  i  .2.  x,0,0 [u,0,0]  0,x,0 [0,u,0]  \tilde{x},x,0 [\tilde{u},u,0]  \\
\tilde{x},0,1/2 [\tilde{u},0,0]  0,\tilde{x},1/2 [0,\tilde{u},0]  x,\tilde{x},1/2 [u,u,0]  \\
\tilde{x},0,0 [\tilde{u},u,0]  0,\tilde{x},0 [0,\tilde{u},0]  x,\tilde{x},0 [u,u,0]  \\
x,0,1/2 [u,0,0]  0,x,1/2 [0,u,0]  \tilde{x},\tilde{x},1/2 [\tilde{u},\tilde{u},0]  \\
6  h  m'm'2  x,2x,1/4 [u,2u,0]  2x,\tilde{x},1/4 [2u,\tilde{u},0]  x,\tilde{x},1/4 [u,u,0]  \\
\tilde{x},2x,3/4 [\tilde{u},2\tilde{u},0]  2x,\tilde{x},3/4 [2u,\tilde{u},0]  \tilde{x},\tilde{x},3/4 [\tilde{u},\tilde{u},0]  \\
6  g  .2/m'.  1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  1/2,1/2,0 [0,0,0]  \\
1/2,2,1/2 [0,0,0]  0,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  \\
4  f  3m'.  1/3,2/3,z [0,0,w]  2/3,1/3,z+1/2 [0,0,w]  2/3,1/3,z [0,0,\tilde{w}]  \\
1/3,2/3,z+1/2 [0,0,\tilde{w}]  1/3,2/3,z+1/2 [0,0,\tilde{w}]  \\
4  e  3m'.  0,0,z [0,0,w]  0,0,z+1/2 [0,0,w]  0,0,\tilde{z} [0,0,\tilde{w}]  \\
0,0,\tilde{z}+1/2 [0,0,\tilde{w}]  \\
2  d  \bar{6}m'2  1/3,2/3,3/4 [0,0,0]  2/3,1/3,1/4 [0,0,0]  \\
2  c  \bar{6}m'2  1/3,2/3,1/4 [0,0,0]  2/3,1/3,3/4 [0,0,0]  \\
2  b  \bar{6}m'2  0,0,1/4 [0,0,0]  0,0,3/4 [0,0,0]  \\
2  a  \bar{3}m'.  0,0,0 [0,0,0]  0,0,1/2 [0,0,0]  \\

Symmetry of Special Projections

Along [0,0,1]  p6m'm'  
Along [1,0,0]  p2m'g'  
Along [2,1,0]  p2m'm'

a* = a  \quad b* = b 
\quad a* = c  \quad b* = (a + 2b)/2
\quad a* = c/2  \quad b* = b/2

Origin at 0,0,z  
Origin at x,0,0  
Origin at x,x/2,0
Origin at 23

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2; \quad y \leq 1-x; \quad z \leq \min (x,y) \]

Vertices

\[ \begin{align*}
0,0,0 & \quad 1,0,0 \\
0,1,0 & \quad 1/2,1/2,1/2
\end{align*} \]

Symmetry Operations

\[ \begin{align*}
(1) & \quad 1 \\
(10) & \quad 3^+ x,x,x \\
& \quad (3_{xyz})^{-1} |0,0,0|
\end{align*} \]

\[ \begin{align*}
(2) & \quad 2 \quad 0,0,z \\
& \quad (2_z) |0,0,0|
\end{align*} \]

\[ \begin{align*}
(3) & \quad 2 \quad 0,y,0 \\
& \quad (2_y) |0,0,0|
\end{align*} \]

\[ \begin{align*}
(4) & \quad 2 \quad x,0,0 \\
& \quad (2_x) |0,0,0|
\end{align*} \]

\[ \begin{align*}
(5) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}) |0,0,0|
\end{align*} \]

\[ \begin{align*}
(6) & \quad 3^+ \bar{x},\bar{x},\bar{x} \\
& \quad (3_{xyz})^{-1} |0,0,0|
\end{align*} \]

\[ \begin{align*}
(7) & \quad 3^+ \bar{x},\bar{x},\bar{x} \\
& \quad (3_{xyz})^{-1} |0,0,0|
\end{align*} \]

\[ \begin{align*}
(8) & \quad 3^+ \bar{x},\bar{x},x \\
& \quad (3_{xyz})^{-1} |0,0,0|
\end{align*} \]

Continued

\[ \begin{align*}
(11) & \quad 3^- \bar{x},\bar{x},x \\
& \quad (3_{xyz}) |0,0,0|
\end{align*} \]

\[ \begin{align*}
(12) & \quad 3^- \bar{x},\bar{x},\bar{x} \\
& \quad (3_{xyz}) |0,0,0|
\end{align*} \]
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 j 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) (z,\bar{x},\bar{y} [w,\bar{u},\bar{v}])</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) (\bar{y},\bar{z},x [v,w,\bar{u}])</td>
</tr>
</tbody>
</table>

6 i 2.. x,1/2,1/2 [u,0,0] \(\bar{x},1/2,1/2 [\bar{u},0,0]\) 1/2,x,1/2 [0,u,0] 1/2,0,x [0,0,u] 1/2,x,0 [0,u,0] 0,1/2,x [0,0,u] 0,1/2,\(\bar{x}\) [0,0,\(\bar{u}\)]

6 h 2.. x,1/2,0 [u,0,0] \(\bar{x},1/2,0 [\bar{u},0,0]\) 0,x,1/2 [0,u,0] 0,\(\bar{x}\),1/2 [0,0,\(\bar{u}\)] 1/2,0,x [0,0,u] 0,1/2,x [0,0,u] 0,1/2,\(\bar{x}\) [0,0,\(\bar{u}\)]

6 g 2.. x,0,1/2 [u,0,0] \(\bar{x},0,1/2 [\bar{u},0,0]\) 1/2,x,0 [0,u,0] 0,1/2,x [0,0,u] 0,1/2,\(\bar{x}\) [0,0,\(\bar{u}\)] 0,0,x [0,u,0] 0,0,\(\bar{x}\) [0,0,\(\bar{u}\)]

6 f 2.. x,0,0 [u,0,0] \(\bar{x},0,0 [\bar{u},0,0]\) 0,x,0 [0,u,0] 0,0,x [0,u,0] 0,0,\(\bar{x}\) [0,0,\(\bar{u}\)] 0,0,\(\bar{x}\) [0,0,\(\bar{u}\)]

4 e .3. x,x,x [u,u,u] \(\bar{x},\bar{x},\bar{x} [\bar{u},\bar{u},\bar{u}]\) \(\bar{x},x,\bar{x} [\bar{u},u,u]\) \(\bar{x},x,\bar{x} [\bar{u},\bar{u},u]\) \(\bar{x},x,\bar{x} [\bar{u},\bar{u},\bar{u}]\)

3 d 222.. 1/2,0,0 [0,0,0] 0,1/2,0 [0,0,0] 0,0,1/2 [0,0,0]

3 c 222.. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]

1 b 23. 1/2,1/2,1/2 [0,0,0]

1 a 23. 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2m1'm'
\(a^* = a\) \(b^* = b\)
Origin at 0,0,z

Along [1,1,1] p3
\(a^* = (2a - b - c)/3\) \(b^* = (-a + 2b - c)/3\)
Origin at x,x,x

Along [1,1,0] p1m1'
\(a^* = (-a + b)/2\) \(b^* = c\)
Origin at x,x,0
Origin at 231'

Asymmetric unit

\[0 \leq x \leq 1; \quad 0 \leq y \leq 1; \quad 0 \leq z \leq 1/2; \quad y \leq 1-x; \quad z \leq \min (x,y)\]

Vertices

\[0,0,0 \quad 1,0,0 \quad 0,1,0 \quad 1/2,1/2,1/2\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1,0,0) \\
(5) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}|0,0,0) \\
(9) & \quad 3^- x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(2) & \quad 2,0,0 \\
(2) & \quad (2,0,0,0) \\
(6) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(10) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}|0,0,0) \\
(3) & \quad 0,y,0 \\
(3) & \quad (2,0,0,0) \\
(7) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(11) & \quad 3^- x,x,x \\
& \quad (3_{xyz}|0,0,0) \\
(4) & \quad 2,x,0 \\
(4) & \quad (2,0,0,0) \\
(8) & \quad 3^- x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(12) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}|0,0,0)
\end{align*}
\]
For 1' + set

(1) 1' (1 [0,0,0])
(2) 2' 0,0,z
    (2 [0,0,0])
(3) 2' 0,y,0
    (2 [0,0,0])
(4) 2' x,0,0
    (2 [0,0,0])

(5) 3' x,x,x
    (3 [0,0,0])
(6) 3' x,x,x
    (3 [0,0,0])
(7) 3' x,x,x
    (3 [0,0,0])
(8) 3' x,x,x
    (3 [0,0,0])

(9) 3' x,x,x
    (3 [0,0,0])
(10) 3' x,x,x
    (3 [0,0,0])
(11) 3' x,x,x
    (3 [0,0,0])
(12) 3' x,x,x
    (3 [0,0,0])

Generators selected
(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5): 1'.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>1 + 1' +</td>
</tr>
<tr>
<td>12 j 11'</td>
<td>1 + 1' +</td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(5) x,y,z [0,0,0]</td>
<td>(6) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(9) y,z,x [0,0,0]</td>
<td>(10) y,z,x [0,0,0]</td>
</tr>
</tbody>
</table>

| 6 i 2..1' | x,1/2,1/2 [0,0,0] |
| 1/2 x,1/2 [0,0,0] | 1/2 x,1/2 [0,0,0] |
| 1/2 1/2 x,1/2 [0,0,0] | 1/2 1/2 x,1/2 [0,0,0] |
| (1) x,1/2,1/2 [0,0,0] | (2) x,1/2,1/2 [0,0,0] | (3) x,1/2,1/2 [0,0,0] | (4) x,1/2,1/2 [0,0,0] |

| 6 h 2..1' | x,1/2,0 [0,0,0] |
| 0,1/2 x,1/2 [0,0,0] | 0,1/2 x,1/2 [0,0,0] |
| 1/2 0,1/2 [0,0,0] | 1/2 0,1/2 [0,0,0] |
| (1) x,1/2,0 [0,0,0] | (2) x,1/2,0 [0,0,0] | (3) x,1/2,0 [0,0,0] | (4) x,1/2,0 [0,0,0] |

| 6 g 2..1' | x,0,1/2 [0,0,0] |
| 1/2 x,0,1/2 [0,0,0] | 1/2 x,0,1/2 [0,0,0] |
| 0,1/2 x,0,1/2 [0,0,0] | 0,1/2 x,0,1/2 [0,0,0] |
| (1) x,0,1/2 [0,0,0] | (2) x,0,1/2 [0,0,0] | (3) x,0,1/2 [0,0,0] | (4) x,0,1/2 [0,0,0] |

| 6 f 2..1' | x,0,0 [0,0,0] |
| 0,0 x,0 [0,0,0] | 0,0 x,0 [0,0,0] |
| 0,0,0 x,0 [0,0,0] | 0,0,0 x,0 [0,0,0] |
| (1) x,0,0 [0,0,0] | (2) x,0,0 [0,0,0] | (3) x,0,0 [0,0,0] | (4) x,0,0 [0,0,0] |

| 4 e .3.1' | x,x,x [0,0,0] |
| x,x,x [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |
| (1) x,x,x [0,0,0] | (2) x,x,x [0,0,0] | (3) x,x,x [0,0,0] | (4) x,x,x [0,0,0] |

| 3 d 222..1' | 1/2,0,0 [0,0,0] |
| 0,1/2,0 [0,0,0] | 0,1/2,0 [0,0,0] |
| 0,0,1/2 [0,0,0] | 0,0,1/2 [0,0,0] |
| (1) 1/2,0,0 [0,0,0] | (2) 1/2,0,0 [0,0,0] | (3) 1/2,0,0 [0,0,0] | (4) 1/2,0,0 [0,0,0] |

| 3 c 222..1' | 0,1/2,1/2 [0,0,0] |
| 1/2,0,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |
| 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| (1) 0,1/2,1/2 [0,0,0] | (2) 0,1/2,1/2 [0,0,0] | (3) 0,1/2,1/2 [0,0,0] | (4) 0,1/2,1/2 [0,0,0] |

| 1 b 23.1 | 1/2,1/2,1/2 [0,0,0] |
| 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |
| 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |
| (1) 1/2,1/2,1/2 [0,0,0] | (2) 1/2,1/2,1/2 [0,0,0] | (3) 1/2,1/2,1/2 [0,0,0] | (4) 1/2,1/2,1/2 [0,0,0] |

| 1 a 23.1 | 0,0,0 [0,0,0] |
| 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |
| 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |
| (1) 0,0,0 [0,0,0] | (2) 0,0,0 [0,0,0] | (3) 0,0,0 [0,0,0] | (4) 0,0,0 [0,0,0] |
Symmetry of Special Projections

Along [0,0,1] p2mm1'  
\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]  
Origin at 0,0,z

Along [1,1,1] p31'  
\[ \mathbf{a}^* = \frac{2\mathbf{a} - \mathbf{b} - \mathbf{c}}{3} \quad \mathbf{b}^* = \frac{-\mathbf{a} + 2\mathbf{b} - \mathbf{c}}{3} \]  
Origin at x,x,x

Along [1,1,0] p1m11'  
\[ \mathbf{a}^* = \frac{-(\mathbf{a} + \mathbf{b})}{2} \quad \mathbf{b}^* = \mathbf{c} \]  
Origin at x,x,0
Origin at 23

Asymmetric unit

0 ≤ x ≤ 1; 0 ≤ y ≤ 1; 0 ≤ z ≤ 1/2; y ≤ 1-x; z ≤ min (x,y)

Vertices
0,0,0 1,0,0 0,1,0 1/2,1/2,1/2

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)
(2) 2 0,0,z (2z|0,0,0)
(3) 2 0,y,0 (2y|0,0,0)
(4) 2 x,0,0 (2x|0,0,0)

(5) 3’ x,x,x (3xyz|0,0,0)
(6) 3’ x,x,x (3xyz^-1|0,0,0)
(7) 3’ x,x,x (3xyz|0,0,0)
(8) 3’ x,x,x (3xyz^-1|0,0,0)

(9) 3’ x,x,x (3xyz^-1|0,0,0)
(10) 3’ x,x,x (3xyz|0,0,0)
(11) 3’ x,x,x (3xyz^-1|0,0,0)
(12) 3’ x,x,x (3xyz|0,0,0)
For \( (1,0,0)' + \) set

\[
\begin{align*}
(1) \ t' (1,0,0) & \quad (2) \ 2' 1/2,0,z \\
(1'1,0,0)' & \quad (3) \ 2' 1/2,y,0 \\
(2'1,0,0)' & \quad (4) \ 2' (1,0,0) x,0,0 \\
(2'1,0,0)' & \quad (2'1,0,0)' \\
(5) \ 3' (1/3,1/3,1/3) & \quad (6) \ 3' (1/3,-1/3,1/3) \\
x+2/3,x+1/3,x & \quad (7) \ 3' (1/3,-1/3,-1/3) \\
(3_{xyz}|1,0,0)' & \quad (3_{xyz}-1|1,0,0)' \\
(5) \ 3' (1/3,1/3,1/3) & \quad (9) \ 3' (1/3,1/3,1/3) \\
x+1/3,x+1/3,x & \quad (12) \ 3' (1/3,1/3,1/3) \\
(3_{xyz}-1|1,0,0)' & \quad (3_{xyz}|1,0,0)' \\
(3_{xyz}-1|1,0,0)' & \quad (3_{xyz}|1,0,0)' \\
(3_{xyz}-1|1,0,0)' & \quad (3_{xyz}-1|1,0,0)' \\
(Generators selected) & \quad (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5).
\end{align*}
\]

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>(0,0,0) + (1,0,0)' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(x,1/2,1/2 [u,0,0])</td>
</tr>
<tr>
<td>(2) (\bar{x},\bar{y},\bar{z} [u,v,w])</td>
<td>(\bar{x},1/2,1/2 [u,0,0])</td>
</tr>
<tr>
<td>(3) (x,y,z [u,v,w])</td>
<td>(x,1/2,1/2 [u,0,0])</td>
</tr>
<tr>
<td>(4) (x,y,z [u,v,w])</td>
<td>(x,1/2,1/2 [u,0,0])</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
12 & \quad i \quad 2'. \quad x,1/2,1/2 [u,0,0] \\
& \quad 1/2 , x,1/2 [0,u,0] \\
& \quad 1/2,1/2,x [0,0,u] \\
& \quad 1/2,1/2 , x [0,0,u] \\
12 & \quad h \quad 2'. \quad x,1/2,0 [0,v,w] \\
& \quad 0,x,1/2 [0,0,v] \\
& \quad 0,1/2,x [v,w,0] \\
& \quad 1/2,0 , x [v,w,0] \\
12 & \quad g \quad 2'. \quad x,0,1/2 [0,v,w] \\
& \quad 1/2 , x,0 [w,0,v] \\
& \quad 0,1/2,x [v,w,0] \\
& \quad 0,1/2 , x [v,w,0] \\
12 & \quad f \quad 2'. \quad x,0,0 [u,0,0] \\
& \quad 0,x,0 [u,0,0] \\
& \quad 0,0,x [u,0,0] \\
& \quad 0,0 , x [u,0,0] \\
8 & \quad e \quad 3. \quad x,x,x [u,u,u] \\
& \quad x,x,x [u,u,u] \\
& \quad x,x,x [u,u,u] \\
& \quad x,x,x [u,u,u] \\
6 & \quad d \quad 22'. \quad 1/2,0,0 [u,0,0] \\
& \quad 0,1/2,0 [u,0,0] \\
& \quad 0,0,1/2 [0,u,0] \\
& \quad 0,0,1/2 [0,u,0] \\
6 & \quad c \quad 22'. \quad 0,1/2,1/2 [u,0,0] \\
& \quad 1/2,0,1/2 [0,u,0] \\
& \quad 1/2,1/2,0 [0,u,0] \\
& \quad 1/2,1/2,0 [0,u,0] \\
2 & \quad b \quad 23. \quad 1/2,1/2,1/2 [0,0,0] \\
2 & \quad a \quad 23. \quad 0,0,0 [0,0,0] \\
\end{align*}
\]
# Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Group</th>
<th>Formulae</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p2mm1'</td>
<td>( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} )</td>
<td>0,0,z</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \mathbf{a}^* = \frac{(2\mathbf{a} - \mathbf{b} - \mathbf{c})}{3} ) \quad \mathbf{b}^* = \frac{(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})}{3}</td>
<td>x,x,x</td>
</tr>
<tr>
<td>Along [1,1,1]</td>
<td>p31'</td>
<td>( \mathbf{a}^* = \frac{(-\mathbf{a} + \mathbf{b})}{2} ) \quad \mathbf{b}^* = \mathbf{c}</td>
<td>x-1/4,x+1/4,0</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p(_c).1m1</td>
<td>( \mathbf{a}^* = \frac{(-\mathbf{a} + \mathbf{b})}{2} ) \quad \mathbf{b}^* = \mathbf{c}</td>
<td>x-1/4,x+1/4,0</td>
</tr>
</tbody>
</table>
Origin at 23

Asymmetric unit: $0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad y \leq x; \quad \max(x-1/2,-y) \leq z \leq \min(1/2 - x,y)$

Vertices: $0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
2. $2 \times 0,0,z$
   2. $2 \times 0,0,0$
3. $2 \times 0,y,0$
   2. $2 \times 0,0,0$
4. $2 \times x,0,0$
   2. $2 \times 0,0,0$
5. $3^+ x,x,x$
   $3_{xyz}^{-1} 0,0,0$
6. $3^+ x,x,x$
   $3_{xyz}^{-1} 0,0,0$
7. $3^+ x,x,x$
   $3_{xyz}^{-1} 0,0,0$
8. $3^+ x,x,x$
   $3_{xyz}^{-1} 0,0,0$
9. $3^- x,x,x$
   $3_{xyz}^{-1} 0,0,0$
10. $3^- x,x,x$
    $3_{xyz}^{-1} 0,0,0$
11. $3^- x,x,x$
    $3_{xyz}^{-1} 0,0,0$
12. $3^- x,x,x$
    $3_{xyz}^{-1} 0,0,0$
Continued

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (2) 2 (0,0,1/2) 0,1/4,z (3) 2 (0,1/2,0) 0,y,1/4 (4) 2 x,1/4,1/4
   (1 0,1/2,1/2) (2z 0,1/2,1/2) (2z 0,1/2,1/2) (2z 0,1/2,1/2)

(5) 3* (1/3,1/3,1/3) x+1/3,x-1/6,x (3xyz 0,1/2,1/2)
   (6) 3* x,x+1/2,x (7) 3* -1/3,1/3,1/3 x+1/3,x-1/6,x (8) 3* x,x+1/2,x
   (3xyz -1 0,1/2,1/2) (3xyz -1 0,1/2,1/2) (3xyz -1 0,1/2,1/2)

(9) 3* (1/3,1/3,1/3) x+1/6,x+1/6,x (3xyz -1 0,1/2,1/2)
   (10) 3* -1/3,1/3,1/3 x+1/6,x+1/6,x (11) 3* x,x+1/2,x+1/2,x (12) 3* x-1/2,x+1/2,x
   (3xyz -1 0,1/2,1/2) (3xyz -1 0,1/2,1/2) (3xyz -1 0,1/2,1/2)

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2) (2) 2 (0,0,1/2) 1/4,0,z (3) 2 1/4,y,1/4 (4) 2 (1/2,0,0) x,0,1/2
   (1 1/2,0,1/2) (2z 1/2,0,1/2) (2z 1/2,0,1/2) (2z 1/2,0,1/2)

(5) 3* (1/3,1/3,1/3) x+1/6,x-1/6,x (3xyz 1/2,0,1/2)
   (6) 3* x,x+1/2,x (7) 3* x+1/2,x-1/2,x (8) 3* x,x+1/2,x+1/2,x
   (3xyz -1 1/2,0,1/2) (3xyz -1 1/2,0,1/2) (3xyz -1 1/2,0,1/2)

(9) 3* (1/3,1/3,1/3) x+1/6,x+1/3,x (3xyz -1 1/2,0,1/2)
   (10) 3* x,x+1/2,x (11) 3* x,x+1/2,x (12) 3* x,x+1/2,x
   (3xyz -1 1/2,0,1/2) (3xyz -1 1/2,0,1/2) (3xyz -1 1/2,0,1/2)

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (2) 2 1/4,1/4,z (3) 2 (0,1/2,0) 1/4,y,0 (4) 2 (1/2,0,0) x,1/4,0
   (1 1/2,1/2,0) (2z 1/2,1/2,0) (2z 1/2,1/2,0) (2z 1/2,1/2,0)

(5) 3* (1/3,1/3,1/3) x+1/6,x+1/3,x (3xyz 1/2,1/2,0)
   (6) 3* x,x+1/2,x (7) 3* x+1/2,x,x (8) 3* x,x+1/2,x+1/2,x
   (3xyz -1 1/2,1/2,0) (3xyz -1 1/2,1/2,0) (3xyz -1 1/2,1/2,0)

(9) 3* (1/3,1/3,1/3) x+1/3,x+1/6,x (3xyz -1 1/2,1/2,0)
   (10) 3* x,x+1/2,x (11) 3* x,x+1/2,x (12) 3* x,x+1/2,x
   (3xyz -1 1/2,1/2,0) (3xyz -1 1/2,1/2,0) (3xyz -1 1/2,1/2,0)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5).

Positions

Multiplicity, 48
Wyckoff letter, h
Site Symmetry. 1

(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0)

x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]
(5) z,x,y [w,u,v] (6) z,x,y [w,u,v] (7) z,x,y [w,u,v] (8) z,x,y [w,u,v]
(9) y,z,x [v,w,u] (10) y,z,x [v,w,u] (11) y,z,x [v,w,u] (12) y,z,x [v,w,u]
24  g  2..  x,1/4,1/4 [u,0,0]  \[\bar{x},3/4,1/4 \ [\bar{u},0,0]\]  \[1/4,1/4,\bar{x} \ [0,u,0]\]  \\
24  f  2..  x,0,0 [u,0,0]  \[\bar{x},0,0 \ [\bar{u},0,0]\]  \[0,x,0 \ [0,u,0]\]  \\
16  e  .3.  x,x,x [u,u,u]  \[x,x,x \ [\bar{u},\bar{u},\bar{u}]\]  \[x,x,x \ [\bar{u},u,u]\]  \[x,x,x \ [u,u,u]\]  \\
4    d  23.  x,0,0 [u,0,0]  \[0,0,0 \ [0,u,0]\]  \\
4    c  23.  x,0,0 [u,0,0]  \[0,0,0 \ [0,u,0]\]  \\
4    b  23.  x,0,0 [u,0,0]  \[0,0,0 \ [0,u,0]\]  \\
Symmetry of Special Projections  
Along [0,0,1]  p2m'  
Origin at 0,0,z  
\[a^* = a/2 \quad b^* = b/2\]  
Along [1,1,1]  p3  
Origin at x,x,x  
\[a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6\]  
Along [1,1,0]  c1m'  
Origin at x,x,0  
\[a^* = (-a + b)/2 \quad b^* = c\]
**Origin** at 231’

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad y \leq x; \quad \text{max}(x-1/2,-y) \leq z \leq \min (1/2 - x,y) \]

**Vertices**

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>1/2,1/2,0</th>
<th>1/4,1/4,1/4</th>
<th>1/4,1/4,-1/4</th>
</tr>
</thead>
</table>

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \(1\)
   
2. \(2 \quad 0,0,z\)
   
3. \(2 \quad 0,y,0\)
   
4. \(2 \quad x,0,0\)

5. \(3^+ \quad x,x,x\)
   
6. \(3^+ \quad x,x,x\)

7. \(3^+ \quad x,x,x\)
   
8. \(3^+ \quad x,x,x\)

9. \(3^- \quad x,x,x\)
   
10. \(3^- \quad x,x,x\)

11. \(3^- \quad x,x,x\)

12. \(3^- \quad x,x,x\)
Continued

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(2) 2 (0,0,1/2)  0,1/4,z  
(3) 2 (0,1/2,0)  0,y,1/4  
(4) 2 x,1/4,1/4  

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2)  
(2) 2 (0,0,1/2)  1/4,0,z  
(3) 2 1/4,y,1/4  
(4) 2 (1/2,0,0)  x,0,1/2  

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(2) 2 1/4,1/4,z  
(3) 2 (0,1/2,0)  1/4,y,0  
(4) 2 (1/2,0,0)  x,1/4,0  

For (1,2,0,1/2) + set

(1) t (1/2,0,1/2)  
(2) 2 (0,0,1/2)  1/4,0,z  
(3) 2 1/4,y,1/4  
(4) 2 (1/2,0,0)  x,0,1/2  

For (1,2,1/2,0) + set

(1) t (1/2,1/2,0)  
(2) 2 1/4,1/4,z  
(3) 2 (0,1/2,0)  1/4,y,0  
(4) 2 (1/2,0,0)  x,1/4,0  

For (1,2,1/2,0) + set

(1) 1'  
(2) 2' 0,0,z  
(3) 2' 0,y,0  
(4) 2' x,0,0  

For (0,0,0)' + set

(1) 0,0,0)'  
(2) 2' 0,0,z  
(3) 2' 0,y,0  
(4) 2' x,0,0  

(3) xyz 0,0,0)'  
(4) 3* x,x,x  
(5) 3* x,x,x  
(6) 3* x,x,x  
(7) 3* x,x,x  
(8) 3* x,x,x  
(9) 3* x,x,x  
(10) 3* x,x,x  
(11) 3* x,x,x  
(12) 3* x,x,x  

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Continued

For (0,1/2,1/2) + set

(1) t' (0,1/2,1/2)
   (1) [0,1/2,1/2]
(2) 2' (0,0,1/2) 0,1/4,z
(2) z,0,1/2,1/2)
(3) 2' (0,1/2,0) 0,y,1/4
(3) z,0,1/2,1/2)
(4) 2' x,1/4,1/4
(4) z,0,1/2,1/2)
(5) 3' (1/3,1/3,1/3)
   x+1/3,x+1/3,x
(3) [0,1/2,1/2)]
(6) 3' - (1/3,1/3,1/3)
   x+1/3,x+1/3,x
(3) [0,1/2,1/2)]
(7) 3' x+1/2,x+1/2,x
(3) [0,1/2,1/2)]
(8) 3' x+1/2,x+1/2,x
(3) [0,1/2,1/2)]
(9) 3' (1/3,1/3,1/3)
   x+1/6,x+1/6,x
(3) [0,1/2,1/2)]
(10) 3' (1/3,1/3,1/3)
   x+1/6,x+1/6,x
(3) [0,1/2,1/2)]
(11) 3' x+1/6,x+1/6,x
(3) [0,1/2,1/2)]
(12) 3' x+1/6,x+1/6,x
(3) [0,1/2,1/2)]

For (1/2,0,1/2) + set

(1) t' (1/2,0,1/2)
   (1) [1/2,0,1/2)
(2) 2' (0,0,1/2) 1/4,0,z
(2) z,1/2,0,1/2)
(3) 2' 1/4,y,1/4
(3) z,1/2,0,1/2)
(4) 2' (1/2,0,0) x,0,1/2
(4) z,1/2,0,1/2)
(5) 3' (1/3,1/3,1/3)
   x+1/6,x+1/6,x
(3) [1/2,0,1/2)]
(6) 3' (1/3,-1/3,1/3)
   x+1/6,x+1/6,x
(3) [1/2,0,1/2)]
(7) 3' x+1/2,x+1/2,x
(3) [1/2,0,1/2)]
(8) 3' x+1/2,x+1/2,x
(3) [1/2,0,1/2)]
(9) 3' (1/3,1/3,1/3)
   x+1/6,x+1/3,x
(3) [1/2,0,1/2)]
(10) 3' x+1/6,x+1/3,x
(3) [1/2,0,1/2)]
(11) 3' x+1/6,x+1/3,x
(3) [1/2,0,1/2)]
(12) 3' x+1/6,x+1/3,x
(3) [1/2,0,1/2)]

For (1/2,1/2,0) + set

(1) t' (1/2,1/2,0)
   (1) [1/2,1/2,0')
(2) 2' 1/4,1/4,z
(2) z,1/2,1/2,0'
(3) 2' (0,1/2,0) 1/4,y,0
(3) z,1/2,1/2,0'
(4) 2' (1/2,0,0) x,1/4,0
(4) z,1/2,1/2,0'
(5) 3' (1/3,1/3,1/3)
   x+1/6,x+1/3,x
(3) [1/2,1/2,0')
(6) 3' (1/3,-1/3,1/3)
   x+1/6,x+1/3,x
(3) [1/2,1/2,0')
(7) 3' x+1/2,x+1/2,x
(3) [1/2,1/2,0')
(8) 3' x+1/2,x+1/2,x
(3) [1/2,1/2,0')
(9) 3' (1/3,1/3,1/3)
   x+1/3,x+1/6,x
(3) [1/2,1/2,0')
(10) 3' x+1/3,x+1/6,x
(3) [1/2,1/2,0')
(11) 3' x+1/3,x+1/6,x
(3) [1/2,1/2,0')
(12) 3' x+1/3,x+1/6,x
(3) [1/2,1/2,0')

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.
(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
48 h 11'

(1) x,y,z [0,0,0]
(2) x,y,z [0,0,0]
(3) x,y,z [0,0,0]
(4) x,y,z [0,0,0]
(5) z,x,y [0,0,0]
(6) z,x,y [0,0,0]
(7) z,x,y [0,0,0]
(8) z,x,y [0,0,0]
(9) y,z,x [0,0,0]
(10) y,z,x [0,0,0]
(11) y,z,x [0,0,0]
(12) y,z,x [0,0,0]
| 24 | g | 2..1' | x,1/4,1/4 [0,0,0] | x,3/4,1/4 [0,0,0] | 1/4,x,1/4 [0,0,0] |
| 24 | f | 2..1' | x,0,0 [0,0,0] | x,0,0 [0,0,0] | 0,x,0 [0,0,0] |
| 16 | e | .3.1' | x,x,x [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |
| 4  | d | 23.1' | 3/4,3/4,3/4 [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |
| 4  | c | 23.1' | 1/4,1/4,1/4 [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |
| 4  | b | 23.1' | 1/2,1/2,1/2 [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |
| 4  | a | 23.1' | 0,0,0 [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'
- a* = a/2  b* = b/2
- Origin at 0,0,z

Along [1,1,1] p31'
- a* = (2a - b - c)/6  b* = (-a + 2b - c)/6
- Origin at x,x,x

Along [1,1,0] c1m11'
- a* = (-a + b)/2  b* = c
- Origin at x,x,0
Origin at 23

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min(x,1-x); \quad z \leq y \]

Vertices

\(0,0,0\) \quad 1,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 2 \quad 0,y,0 \\
(4) & \quad 2 \quad x,0,0 \\
(5) & \quad 3^+ \quad x,x,x \\
(6) & \quad 3^+ \quad x,x,x \\
(7) & \quad 3^+ \quad x,x,x \\
(8) & \quad 3^+ \quad x,x,x \\
(9) & \quad 3^- \quad x,x,x \\
(10) & \quad 3^- \quad x,x,x \\
(11) & \quad 3^- \quad x,x,x \\
(12) & \quad 3^- \quad x,x,x \\
\end{align*}
\]

\[
\begin{align*}
(1) & \quad (1|0,0,0) \\
(2) & \quad (2z|0,0,0) \\
(3) & \quad (2y|0,0,0) \\
(4) & \quad (2x|0,0,0) \\
(5) & \quad (3_{xyz}^+|0,0,0) \\
(6) & \quad (3_{xyz}^+|0,0,0) \\
(7) & \quad (3_{xyz}^+|0,0,0) \\
(8) & \quad (3_{xyz}^+|0,0,0) \\
(9) & \quad (3_{xyz}^-|0,0,0) \\
(10) & \quad (3_{xyz}^-|0,0,0) \\
(11) & \quad (3_{xyz}^-|0,0,0) \\
(12) & \quad (3_{xyz}^-|0,0,0)
\end{align*}
\]
(1) t (1/2,1/2,1/2) + set

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2) + set

(2) 2 (0,0,1/2) 1/4,1/4,z

(3) 2 (0,1/2,0) 1/4,y,1/4

(4) 2 (1/2,0,0) x,1/4,1/4

(1/2,1/2,1/2) + set

(2a) 1/2,1/2,1/2

(2b) 1/2,1/2,1/2

(3) 2 (0,0,1/2) 1/4,1/4,z

(4) 2 (0,1/2,0) 1/4,y,1/4

(5) 3' (1/2,1/2,1/2) x,x,x

(6) 3' (1/6,-1/6,1/6) x+1/3,x+1/3,x

(7) 3' (-1/6,1/6,1/6) x+2/3,x-1/3,x

(8) 3' (1/6,1/6,-1/6) x+1/3,x+2/3,x

(3xyz 1/2,1/2,1/2)

(3) 2 (0,1/2,0) 1/4,y,1/4

(4) 2 (1/2,0,0) x,1/4,1/4

(2a) 1/2,1/2,1/2

(2b) 1/2,1/2,1/2

(3) 2 (0,1/2,0) 1/4,y,1/4

(4) 2 (1/2,0,0) x,1/4,1/4

Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

24 f 1

(1) x,y,z [u,v,w]

(2) x,y,z [u,v,w]

(3) x,y,z [u,v,w]

(4) x,y,z [u,v,w]

(5) z,x,y [w,u,v]

(6) z,x,y [w,u,v]

(7) z,x,y [w,u,v]

(8) z,x,y [w,u,v]

(9) y,z,x [v,w,u]

(10) y,z,x [v,w,u]

(11) y,z,x [v,w,u]

(12) y,z,x [v,w,u]

12 e 2.. x,1/2,0 [u,0,0] x,1/2,0 [u,0,0]

0,x,1/2 [0,u,0]

0,x,1/2 [0,u,0]

1/2,0,x [0,0,u]

1/2,0,x [0,0,u]

12 d 2.. x,0,0 [u,0,0] x,0,0 [u,0,0]

0,x,0 [0,u,0]

0,x,0 [0,u,0]

0,x,0 [0,u,0]

0,x,0 [0,u,0]

0,x,0 [0,u,0]

8 c .3. x,x,x [u,u,u] x,x,x [u,u,u]

x,x,x [u,u,u]

x,x,x [u,u,u]

x,x,x [u,u,u]

6 b 222.. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]

1/2,1/2,0 [0,0,0]

1/2,1/2,0 [0,0,0]

2 a 23. 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2m'm'

a* = a

b* = b

Origin at 0,0,z

Along [1,1,1] p3

a* = (2a - b - c)/3

b* = (-a + 2b - c)/3

Origin at x,x,x

Along [1,1,0] p1m'1

a* = -(a + b)/2

b* = c/2

Origin at x,x,0

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Origin at 231°
Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min(x, 1-x); \quad z \leq y \]

Vertices

- 0,0,0
- 1,0,0
- 1/2,1/2,0
- 1/2,1/2,1/2

Symmetry Operations

For \((0,0,0) + \text{set}\n
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(1) & \quad 0,0,0 \\
(2) & \quad 2,0,0 \\
(2) & \quad 0,0,0 \\
(3) & \quad 2,0,0 \\
(3) & \quad 0,0,0 \\
(4) & \quad 2,0,0 \\
(4) & \quad 0,0,0 \\
(5) & \quad 3^+ x,x,x \\
(5) & \quad (3_{xyz} | 0,0,0) \\
(6) & \quad 3^+ x,x,x \\
(6) & \quad (3_{xyz} | 0,0,0) \\
(7) & \quad 3^+ x,x,x \\
(7) & \quad (3_{xyz} | 0,0,0) \\
(8) & \quad 3^- x,x,x \\
(8) & \quad (3_{xyz}^{-1} | 0,0,0) \\
(9) & \quad 3^- x,x,x \\
(9) & \quad (3_{xyz}^{-1} | 0,0,0) \\
(10) & \quad 3^- x,x,x \\
(10) & \quad (3_{xyz}^{-1} | 0,0,0) \\
(11) & \quad 3^- x,x,x \\
(11) & \quad (3_{xyz}^{-1} | 0,0,0) \\
(12) & \quad 3^- x,x,x \\
(12) & \quad (3_{xyz}^{-1} | 0,0,0) \\
\end{align*}
Continued

For (1/2,1/2,1/2) + set

<table>
<thead>
<tr>
<th>(1) t (1/2,1/2,1/2)</th>
<th>(2) t (0,0,1/2)</th>
<th>(3) t (0,1/2,0)</th>
<th>(4) t (1/2,0,0)</th>
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</thead>
<tbody>
<tr>
<td>(1 1/2,1/2,1/2)</td>
<td>1/4,1/4,z</td>
<td>1/4,y,1/4</td>
<td>x,1/4,1/4</td>
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<tr>
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<td></td>
<td>(2 1/2,1/2,1/2)</td>
<td></td>
</tr>
<tr>
<td>2 (1,1/2,1/2)</td>
<td>(2 1/2,1/2,1/2)</td>
<td></td>
<td>(2 1/2,1/2,1/2)</td>
</tr>
</tbody>
</table>

(5) 3' (1/2,1/2,1/2) x,x,x

| (3xyz|1/2,1/2,1/2) |
| (3xyz|1/2,1/2,1/2) |

(9) 3' (1/2,1/2,1/2) x,x,x

For (0,0,0)' + set

<table>
<thead>
<tr>
<th>(1) 1'</th>
<th>(2) 2'</th>
<th>(3) 2'</th>
<th>(4) 2'</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>0,0,0</td>
<td>0,0,0</td>
<td>0,0,0</td>
</tr>
<tr>
<td>(1 0,0,0)'</td>
<td>(2 0,0,0)'</td>
<td>(2 0,0,0)'</td>
<td>(2 0,0,0)'</td>
</tr>
</tbody>
</table>

(5) 3' x,x,x (3xyz|0,0,0)' (3xyz|0,0,0)' (3xyz|0,0,0)' (3xyz|0,0,0)'

(9) 3' x,x,x (3xyz|0,0,0)'

For (1/2,1/2,1/2)' + set

<table>
<thead>
<tr>
<th>(1) t' (1/2,1/2,1/2)</th>
<th>(2) t' (0,0,1/2)</th>
<th>(3) t' (0,1/2,0)</th>
<th>(4) t' (1/2,0,0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1 1/2,1/2,1/2)'</td>
<td>1/4,1/4,z</td>
<td>1/4,y,1/4</td>
<td>x,1/4,1/4</td>
</tr>
<tr>
<td>2 (1/2,1/2,1/2)'</td>
<td></td>
<td>(2 1/2,1/2,1/2)'</td>
<td></td>
</tr>
<tr>
<td>2 (1,1/2,1/2)'</td>
<td>(2 1/2,1/2,1/2)'</td>
<td></td>
<td>(2 1/2,1/2,1/2)'</td>
</tr>
</tbody>
</table>

(5) 3' x,x,x (3xyz|1/2,1/2,1/2)' (3xyz|1/2,1/2,1/2)' (3xyz|1/2,1/2,1/2)' (3xyz|1/2,1/2,1/2)'

(9) 3' x,x,x (3xyz|1/2,1/2,1/2)'

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td>24   f 11'</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
</tr>
</tbody>
</table>

(1) x,y,z [0,0,0] (2) x,y,z [0,0,0] (3) x,y,z [0,0,0] (4) x,y,z [0,0,0]

(5) z,x,y [0,0,0] (6) z,x,y [0,0,0] (7) z,x,y [0,0,0] (8) z,x,y [0,0,0]

(9) y,z,x [0,0,0] (10) y,z,x [0,0,0] (11) y,z,x [0,0,0] (12) y,z,x [0,0,0]

197.2.1509 - 2 - 3340
12  e  2..1'  x,1/2,0 [0,0,0]  x,1/2,0 [0,0,0]  0,x,1/2 [0,0,0]  0,x,1/2 [0,0,0]  
0,x,1/2 [0,0,0]  1/2,0,x [0,0,0]  1/2,0,x [0,0,0]  
12  d  2..1'  x,0,0 [0,0,0]  x,0,0 [0,0,0]  0,x,0 [0,0,0]  0,x,0 [0,0,0]  
0,x,0 [0,0,0]  0,0,x [0,0,0]  0,0,x [0,0,0]  
8  c  .3.1'  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  
6  b  222..1'  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0] 
2  a  23.1'  0,0,0 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1]  c2mm1'  
\[ a^* = a \text{  } b^* = b \]  
Origin at 0,0,z 

Along [1,1,1]  p31'  
\[ a^* = (2a - b - c)/3 \text{  } b^* = (-a + 2b - c)/3 \]  
Origin at x,x,x 

Along [1,1,0]  p1m11'  
\[ a^* = (-a + b)/2 \text{  } b^* = c/2 \]  
Origin at x,x,0
Origin at 23

Asymmetric unit

\[
0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min(x, 1-x); \quad z \leq y
\]

Vertices

\[
0,0,0 \quad 1,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2
\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2) & \quad (2,0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(3) & \quad (2,0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(4) & \quad (2,0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz}^+|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
(6) & \quad (3_{xyz}^+|0,0,0) \\
(7) & \quad 3^+ \quad x,x,\bar{x} \\
(7) & \quad (3_{xyz}^+|0,0,0) \\
(8) & \quad 3^+ \quad \bar{x},x,x \\
(8) & \quad (3_{xyz}^+|0,0,0) \\
(9) & \quad 3^- \quad x,x,x \\
(9) & \quad (3_{xyz}^-|0,0,0) \\
(10) & \quad 3^- \quad x,x,x \\
(10) & \quad (3_{xyz}^-|0,0,0) \\
(11) & \quad 3^- \quad \bar{x},x,\bar{x} \\
(11) & \quad (3_{xyz}^-|0,0,0) \\
(12) & \quad 3^- \quad \bar{x},x,x \\
(12) & \quad (3_{xyz}^-|0,0,0)
\end{align*}
\]
Continued

For \((1/2,1/2,1/2)'\) + set

(1) \(t' (1/2,1/2,1/2)\)
(2) \(2' (0,0,1/2)\)
(3) \(2' (0,1/2,0)\)
(4) \(2' (1/2,0,0)\)
(1/2,1/2,1/2)'

(5) \(3' '(1/2,1/2,1/2)\)
(6) \(3' '(1/6,-1/6,1/6)\)
(7) \(3' '(-1/6,1/6,1/6)\)
(8) \(3' '(1/6,1/6,-1/6)\)

(9) \(3' '(1/2,1/2,1/2)\)
(10) \(3' '(-1/6,1/6,1/6)\)
(11) \(3' '(1/6,1/6,-1/6)\)
(12) \(3' '(1/6,-1/6,1/6)\)

Generators selected (1); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t'(1/2,1/2,1/2)\); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 f 1

\((0,0,0) + (1/2,1/2,1/2)' +\)

\(1) x,y,z [u,v,w]\)
\(2) \bar{x} ,\bar{y} ,z [\bar{u} ,\bar{v} ,\bar{w}]\)
\(3) \bar{x} ,y,z [\bar{u} ,v,w]\)
\(4) x,y,\bar{z} [u,v,\bar{w}]\)

\(5) z,x,y [w,u,v]\)
\(6) \bar{z} ,\bar{x} ,y [\bar{w} ,\bar{u} ,\bar{v}]\)
\(7) \bar{z} ,x,y [\bar{w} ,u,v]\)
\(8) \bar{z} ,x,\bar{y} [\bar{w} ,u,\bar{v}]\)

\(9) y,z,x [v,w,u]\)
\(10) \bar{y} ,z,x [\bar{v} ,\bar{w} ,\bar{u}]\)
\(11) \bar{y} ,\bar{z} ,x [\bar{v} ,\bar{w} ,\bar{u}]\)
\(12) y,z,\bar{x} [v,w,\bar{u}]\)

Symmetry of Special Projections

Along \([0,0,1]\) \(c_p,2m'm'\)
Along \([1,1,1]\) \(p31'\)
Along \([1,1,0]\) \(p_{2\bar{1}} ,1m'1\)

\(a^* = a\)
\(b^* = b\)
\(a^* = (2a-b-c)/3\)
\(b^* = (-a+2b-c)/3\)
\(a^* = (-a+b)/2\)
\(b^* = c/2\)

Origin at \(0,0,z\)
Origin at \(x,x,x\)
Origin at \(x,x,0\)
Origin on 3 [1,1,1] at midpoint of three non-intersecting pairs of parallel 2₁₁ axes

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; -1/2 ≤ z ≤ 1/2; max(x-1/2,-y) ≤ z ≤ min (x,y)

Vertices
0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/2,1/2,1/2 0,1/2,-1/2

Symmetry Operations

(1) 1
(1) 0,0,0

(5) 3⁺ x,x,x
(3_xyz | 0,0,0)

(9) 3⁻ x,x,x
(3_xyz⁻¹ | 0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z
(2_x | 1/2,0,1/2)

(6) 3⁺ x+1/2,x,x⁻
(3_xyz⁻¹ | 1/2,1/2,0)

(10) 3⁻ (-1/3,1/3,1/3)
x+1/6,x+1/6,x
(3_xyz | 0,1/2,1/2)

(3) 2 (0,1/2,0) 0,y,1/4
(2_y | 0,1/2,1/2)

(7) 3⁺ x+1/2,x⁻,-1/2,x⁻
(3_xyz⁻¹ | 1/2,0,1/2)

(11) 3⁻ (1/3,1/3,-1/3)
x+1/3,x+1/6,x
(3_xyz⁻¹ | 1/2,1/2,0)

(4) 2 (1/2,0,0) x,1/4,0
(1/2,1/2,0)

(8) 3⁺ x,x+1/2,x
(3_xyz⁻¹ | 0,1/2,1/2)

(12) 3⁻ (1/3,-1/3,1/3)
x-1/6,x+1/3,x
(3_xyz | 1/2,0,1/2)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 b 1</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) z+1/2,x+1/2,y [w,u,v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) y+1/2,z,z+1/2 [v,w,u]</td>
</tr>
<tr>
<td>4 a .3. x,x,x [u,u,u]</td>
<td>x+1/2,x,x+1/2 [u,u,u]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p2g'g'  Along [1,1,1] p3  Along [1,1,0] p1g'1
a* = a  b* = b  a* = (2a - b - c)/3  b* = (-a + 2b - c)/3  a* = (-a + b)/2  b* = c
Origin at 1/4,0,z  Origin at x,x,x  Origin at x+1/4,x,0
Origin on \(31' [1,1,1]\) at midpoint of three non-intersecting pairs of parallel \(2_1\) axes

Asymmetric unit: \(0 \leq x \leq 1/2;\) \(0 \leq y \leq 1/2;\) \(-1/2 \leq z \leq 1/2;\) \(\max(x-1/2,-y) \leq z \leq \min(x,y)\)

Vertices: 
- \(0,0,0\)
- \(1/2,0,0\)
- \(1/2,1/2,0\)
- \(1/2,1/2,1/2\)
- \(0,1/2,-1/2\)

Symmetry Operations

For \(1 + \) set

1. \(1\) (1) \(1\) (0,0,0)
   (1) \(1\) (0,0,0)

2. \(2\) \((0,0,1/2)\) \(1/4,0,z\)
   \((2)\) \(1/2,0,1/2\)

3. \(2\) \((0,1/2,0)\) \(0,y,1/4\)
   \((2)\) \(0,1/2,1/2\)

4. \(2\) \((1/2,0,0)\) \(x,1/4,0\)
   \((2)\) \(1/2,1/2,0\)

5. \(3^+\) \(x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)

6. \(3^+\) \(
   \frac{x+1/2,x}{(3_{xyz}^{-1}|2,1/2,0)}\)

7. \(3^+\) \(
   \frac{x+1/2,x-1/2}{(3_{xyz}^{-1}|2,0,1/2)}\)

8. \(3^+\) \(
   \frac{x,x+1/2,x}{(3_{xyz}^{-1}|0,1/2,1/2)}\)

9. \(3^-\) \(x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)

10. \(3^-\) \(
    \frac{(-1/3,1/3,1/3)}{x+1/6,x+1/6,x}
    \(3_{xyz}^{-1}|0,1/2,1/2)\)

11. \(3^-\) \(
    \frac{1/3,1/3,-1/3}{x+1/3,x+1/6,x}
    \(3_{xyz}^{-1}|1/2,1/2,0)\)

12. \(3^-\) \(
    \frac{1/3,-1/3,1/3}{x-1/6,x+1/3,x}
    \(3_{xyz}^{-1}|1/2,0,1/2)\)
For 1' + set

(1) 1' (1 | 0, 0, 0)

(2) 2' (0, 0, 1/2) 1/4, 0, z

(3) 2' (0, 1/2, 0) 0, y, 1/4

(4) 2' (1/2, 0, 0) x, 1/4, 0

(5) 3' x, x, x

(6) 3' x + 1/2, x, x

(7) 3' x + 1/2, x - 1/2, x

(8) 3' x, x + 1/2, x

(9) 3' x, x, x

(10) 3' x, y + 1/2, z + 1/2, x + 1/6, x + 1/6, x

(11) 3' x, y + 1/2, z + 1/2, x + 1/3, x + 1/3

(12) 3' x, y + 1/2, z + 1/2, x + 1/3, x + 1/3

Generators selected  (1); t(1, 0, 0); t(0, 1, 0); t(0, 0, 1); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

12 b 11'

(1) x, y, z [0, 0, 0]

(2) x + 1/2, y, z + 1/2 [0, 0, 0]

(3) x, y + 1/2, z + 1/2 [0, 0, 0]

(4) x + 1/2, y + 1/2, z [0, 0, 0]

(5) z, x, y [0, 0, 0]

(6) z + 1/2, x + 1/2, y [0, 0, 0]

(7) z + 1/2, x, y + 1/2 [0, 0, 0]

(8) z, x + 1/2, y + 1/2 [0, 0, 0]

(9) y, z, x [0, 0, 0]

(10) y, z + 1/2, x + 1/2 [0, 0, 0]

(11) y + 1/2, z + 1/2, x [0, 0, 0]

(12) y + 1/2, z, x + 1/2 [0, 0, 0]

4 a .3.1' x, x, x [0, 0, 0] x + 1/2, x, x + 1/2 [0, 0, 0] x + 1/2, x + 1/2, x [0, 0, 0]

Symmetry of Special Projections

Along [0, 0, 1] p2gg1'  Along [1, 1, 1] p31'  Along [1, 1, 0] p1g11'

a* = a  b* = b  a* = (2a - b - c)/3  b* = (-a + 2b - c)/3  a* = (-a + b)/2  b* = c

Origin at 1/4, 0, z  Origin at x, x, x  Origin at x + 1/4, x, 0
Origin on 3 [1,1,1] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 2\textsubscript{1} axes

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min(x,y)\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 0,1/2,0 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \quad (2) & \quad 2 (0,0,1/2) & \quad 1/4,0,z & \quad (3) & \quad 2 (0,1/2,0) & \quad 0,y,1/4 & \quad (4) & \quad 2 (1/2,0,0) & \quad x,1/4,0 \\
& \quad (1|0,0,0) & \quad (2_2|1/2,0,1/2) & \quad (2_3|0,1/2,1/2) & \quad (2_4|1/2,1/2,0)
\end{align*}
\]

\[
\begin{align*}
(5) & \quad 3^+ x,x,x & \quad (6) & \quad 3^+ \bar{x}+1/2,x,\bar{x} & \quad (7) & \quad 3^+ x+1/2,\bar{x}-1/2,\bar{x} & \quad (8) & \quad 3^+ \bar{x},x+1/2,x & \quad (3_{xyz}^{-1}|0,1/2,1/2)
\end{align*}
\]

\[
\begin{align*}
& \quad (3_{xyz}|0,0,0) & \quad (3_{xyz}^{-1}|1/2,1/2,0) & \quad (3_{xyz}^{-1}|1/2,0,1/2) & \quad (3_{xyz}^{-1}|0,1/2,1/2)
\end{align*}
\]

\[
\begin{align*}
(9) & \quad 3^- x,x,x & \quad (10) & \quad 3^- (-1/3,1/3,1/3) & \quad x+1/6, x+1/6, x & \quad (11) & \quad 3^- (1/3,1/3,-1/3) & \quad x+1/3, x+1/6, x & \quad (12) & \quad 3^- (1/3,-1/3,1/3) & \quad x-1/6, x+1/3, x & \quad (3_{xyz}^{-1}|1/2,1/2,0) & \quad (3_{xyz}^{-1}|2,0,1/2)
\end{align*}
\]

\[
\begin{align*}
& \quad (3_{xyz}^{-1}|0,0,0) & \quad (3_{xyz}^{-1}|0,1/2,1/2) & \quad (3_{xyz}^{-1}|2,0,1/2)
\end{align*}
\]
For \((1/2,1/2,1/2)\) + set

\[(1) t(1/2,1/2,1/2)\]
\[(2) 2 \ 0,1/4,z\]
\[(3) 2 \ 1/4,y,0\]
\[(4) 2 \ x,0,1/4\]
\[(1) 1/2,1/2,1/2\]
\[(2) 0,1/2,0\]
\[(2) 1/2,0,0\]
\[(2) 0,0,1/2\]

\[(5) 3^* (1/2,1/2,1/2) \ x,x,x\]
\[(6) 3^* (1/6,-1/6,1/6) \ x-1/6,x+1/3,x\]
\[(7) 3^* (-1/6,1/6,1/6) \ x+1/6,x+1/3,x\]
\[(8) 3^* (1/6,1/6,-1/6) \ x+1/3,x+1/6,x\]

\[(3_{xyz}) 1/2,1/2,1/2\]
\[(3_{xyz}) 0,0,1/2\]
\[(3_{xyz}) 1/2,0,0\]
\[(3_{xyz}) 0,1/2,0\]

\[(5) z,x,y \ [w,u,v]\]
\[(6) z+1/2,x+1/2,y \ [w,u,v]\]
\[(7) x+1/2,z+1/2,y \ [w,u,v]\]
\[(8) z+1/2,x+1/2,w \ [u,v,w]\]

\[(9) y,z,x \ [v,w,u]\]
\[(10) y,z+1/2,x+1/2 \ [v,w,u]\]
\[(11) x+1/2,y+1/2,z+1/2 \ [v,w,u]\]
\[(12) y+1/2,z+1/2,x+1/2 \ [v,w,u]\]

Generators selected \(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 c 1

\[(1) \ x,y,z \ [u,v,w] \quad (2) \ x+1/2,y,z+1/2 \ [\bar{u},\bar{v},\bar{w}] \quad (3) \ x,y+1/2,z+1/2 \ [\bar{u},\bar{v},\bar{w}] \quad (4) \ x+1/2,y+1/2,z \ [u,v,w]\]

\[(5) \ z,x,y \ [w,u,v] \quad (6) \ z+1/2,x+1/2,y \ [w,u,v] \quad (7) \ z+1/2,x,y+1/2 \ [w,u,v] \quad (8) \ z,x+1/2,y+1/2 \ [w,u,v]\]

\[(9) \ y,z,x \ [v,w,u] \quad (10) \ y,z+1/2,x+1/2 \ [v,w,u] \quad (11) \ y+1/2,z+1/2,x \ [v,w,u] \quad (12) \ y+1/2,z,x+1/2 \ [v,w,u]\]

Symmetry of Special Projections

Along \([0,0,1]\) \(c2m'm'\)

\(a^* = a \quad b^* = b\)

Origin at \(1/4,0,z\)

Along \([1,1,1]\) \(p3\)

\(a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3\)

Origin at \(x,x,x\)

Along \([1,1,0]\) \(p1m'1\)

\(a^* = (-a + b)/2 \quad b^* = c/2\)

Origin at \(x,x+1/4,0\)
Origin on 31' [1,1,1] at midpoint of three non-intersecting pairs of parallel 2; axes and of three non-intersecting pairs of parallel 2; axes.

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; z ≤ min (x,y)

Vertices 0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/2,1/2,1/2

Symmetry Operations
For (0,0,0) + set

1
(1 | 0,0,0)

2 (0,0,1/2) 1/4,0,z
(2 | 1/2,0,1/2)

2 (0,1/2,0) 0,y,1/4
(2 | 0,1/2,1/2)

2 (1/2,0,0) x,1/4,0
(2 | 1/2,1/2,0)

(3xyz | 0,0,0)

(3xyz | 1/2,1/2,0)

(7) 3+ x+1/2,x-1/2,x
(3xyz⁻¹ | 1/2,0,1/2)

(8) 3+ x,x+1/2,x
(3xyz⁻¹ | 0,1/2,1/2)

(3xyz | 0,1/2,1/2)

(3xyz | 1/2,1/2,0)

(3xyz | 0,1/2,1/2)

3- x,x,x
(3xyz | 0,0,0)

3+ 3,-x+1/3,-1/3
(3xyz⁻¹ | 1/3,1/3,-1/3)

3+ 3,-x+1/3,-1/3
(3xyz⁻¹ | 1/3,1/3,-1/3)

3+ 3,-x+1/3,-1/3
(3xyz⁻¹ | 1/3,1/3,-1/3)
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(1/2,1/2,1/2) +</th>
<th>(0,0,0)</th>
<th>(1/2,1/2,1/2)' +</th>
</tr>
</thead>
</table>

24 c 11'

(1) x,y,z [0,0,0]  (2) x+1/2,y,z+1/2 [0,0,0]  (3) x,y+1/2,z+1/2 [0,0,0]  (4) x+1/2,y+1/2,z [0,0,0]
(5) z,x,y [0,0,0]  (6) z+1/2,x,y+1/2 [0,0,0]  (7) z+1/2,x,y+1/2 [0,0,0]  (8) z,x+1/2,y+1/2 [0,0,0]
(9) y,z,x [0,0,0]  (10) y,z+1/2,x+1/2 [0,0,0]  (11) y+1/2,z+1/2,x [0,0,0]  (12) y+1/2,z,x+1/2 [0,0,0]
Symmetry of Special Projections

Along [0,0,1] c2mm1'
\[ a^* = a \quad b^* = b \]
Origin at 1/4,0,z

Along [1,1,1] p31'
\[ a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \]
Origin at x,x,x

Along [1,1,0] p1m11'
\[ a^* = (-a + b)/2 \quad b^* = c/2 \]
Origin at x,x+1/4,0

12 b 2..1' x,0,1/4 [0,0,0] \( x + 1/2,0,3/4 [0,0,0] \) 1/4,x,0 [0,0,0]
\( 3/4,x + 1/2,0 [0,0,0] \) 0,1/4,x [0,0,0] \( 0,3/4,x + 1/2 [0,0,0] \)

8 a .3.1' x,x,x [0,0,0] \( x + 1/2,x + 1/2 [0,0,0] \) \( x,x + 1/2,x + 1/2 \) \( x + 1/2,x x + 1/2,x [0,0,0] \)

Along [0,0,1] c2mm1'
Along [1,1,1] p31'
Along [1,1,0] p1m11'

\( a^* = a \quad b^* = b \)
\( a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \)
\( a^* = (-a + b)/2 \quad b^* = c/2 \)
Origin on 3 [1,1,1] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 21 axes

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min(x,y) \]

Vertices

\[ (0,0,0) \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2 \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 2 (0,0,1/2) \quad 1/4,0,z \\
(2) & \quad (2_z) \quad 1/2,0,1/2 \\
(3) & \quad 2 (0,1/2,0) \quad 0,y,1/4 \\
(3) & \quad (2_y) \quad 0,1/2,1/2 \\
(4) & \quad 2 (1/2,0,0) \quad x,1/4,0 \\
(4) & \quad (2_x) \quad 1/2,1/2,0 \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz}) \quad 0,0,0 \\
(6) & \quad 3^+ \quad x+1/2, 0, z \\
(6) & \quad (3_{xyz})^{-1} \quad 1/2,1/2,0 \\
(7) & \quad 3^+ \quad x+1/2, x-1/2, x \\
(7) & \quad (3_{xyz})^{-1} \quad 1/2,0,1/2 \\
(8) & \quad 3^+ \quad x, x+1/2, x \\
(8) & \quad (3_{xyz})^{-1} \quad 0,1/2,1/2 \\
(9) & \quad 3^- \quad x,x,x \\
(9) & \quad (3_{xyz})^{-1} \quad 0,0,0 \\
(10) & \quad 3^- \quad -1/3,1/3,1/3 \\
(10) & \quad x+1/6, x+1/6, x \\
& \quad (3_{xyz}) \quad 0,1/2,1/2 \\
(11) & \quad 3^- \quad 1/3,1/3,-1/3 \\
(11) & \quad x+1/3, x+1/6, x \\
& \quad (3_{xyz}) \quad 1/2,1/2,0 \\
(12) & \quad 3^- \quad 1/3,-1/3,1/3 \\
(12) & \quad x-1/6, x+1/3, x \\
& \quad (3_{xyz}) \quad 1/2,0,1/2 \\
\end{align*}
\]
Continued

For \((1/2,1/2,1/2)'\) + set

(1) \(t' (1/2,1/2,1/2)
(1 \| 1/2,1/2,1/2)'

(2) \(2' 0,1/4,z
(2_z|0,1/2,0)'

(3) \(2' 1/4,y,0
(2_y|1/2,0,0)'

(4) \(2' x,0,1/4
(2_x|0,0,1/2)'

(5) \(3+ ' (1/2,1/2,1/2) x,x,x
(5 \| 1/2,1/2,1/2)'

(6) \(3+ ' (1/6,-1/6,1/6)
(3_yz|1/2,1/2,1/2)'

(7) \(3+ ' (1/6,1/6,-1/6)
(3_xz|1/2,1/2,1/2)'

(9) \(3- ' (1/2,1/2,1/2) x,x,x
(9 \| 1/2,1/2,1/2)'

Generators selected

(1); \(t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>c 1</td>
<td></td>
</tr>
</tbody>
</table>

(1) \(x,y,z [u,v,w]

(2) \(\bar{x}+1/2,\bar{y},z+1/2 [u,\bar{v},w]

(3) \(x,y+1/2,\bar{z}+1/2 [u,v,\bar{w}]

(4) \(x+1/2,\bar{y}+1/2,\bar{z} [u,\bar{v},\bar{w}]

(5) \(z,x,y [w,u,v]

(6) \(z+1/2,\bar{x}+1/2,\bar{y} [w,u,\bar{v}]

(7) \(\bar{z}+1/2,\bar{x},y+1/2 [\bar{w},u,v]

(8) \(\bar{z},x+1/2,\bar{y}+1/2 [w,u,\bar{v}]

(9) \(y,z,x [v,w,u]

(10) \(\bar{y},z+1/2,\bar{x}+1/2 [\bar{v},w,u]

(11) \(y+1/2,\bar{z}+1/2,\bar{x} [v,w,u]

(12) \(y+1/2,\bar{z},x+1/2 [\bar{v},w,u]

Symmetry of Special Projections

Along \([0,0,1]\) \(c_{p}2\text{mm}\) Along \([1,1,1]\) \(p31'\) Along \([1,1,0]\) \(p_{2b}.1\text{m}1\)

\(a^{*} = a\) \(b^{*} = b\) \(a^{*} = (2a - b - c)/3\) \(b^{*} = (-a + 2b - c)/3\) \(a^{*} = (-a + b)/2\) \(b^{*} = c/2\)

Origin at \(1/4,0,z\) Origin at \(x,x,x\) Origin at \(x,x+1/4,0\)
Origin at center \((m\bar{3})\)

Asymmetric unit:

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min (x,y)
\]

Vertices:

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 0,1/2,0 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations:

1. \(1\)
   - \((1 \mid 0,0,0)\)

2. \(2\)
   - \((0,0,z)\)
   - \((0,0,0)\)

3. \(2\)
   - \((0,y,0)\)
   - \((0,0,0)\)

4. \(2\)
   - \((x,0,0)\)
   - \((0,0,0)\)

5. \(3^{+}\)
   - \((x,x,x)\)
   - \((0,0,0)\)

6. \(3^{+}\)
   - \((x,x,x)\)
   - \((0,0,0)\)

7. \(3^{+}\)
   - \((x,x,x)\)
   - \((0,0,0)\)

8. \(3^{+}\)
   - \((x,x,x)\)
   - \((0,0,0)\)

9. \(3^{-}\)
   - \((x,x,x)\)
   - \((0,0,0)\)

10. \(3^{-}\)
    - \((x,x,x)\)
    - \((0,0,0)\)

11. \(3^{-}\)
    - \((x,x,x)\)
    - \((0,0,0)\)

12. \(3^{-}\)
    - \((x,x,x)\)
    - \((0,0,0)\)

Continued
<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
<th>Coordinates</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$x,y,z$ ([u,v,w])</td>
<td>$x,y,z$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>2</td>
<td>$x,x,x$ ([u,u,u])</td>
<td>$x,x,x$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>3</td>
<td>$x,y,z$ ([u,v,w])</td>
<td>$x,y,z$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>4</td>
<td>$x,y,z$ ([u,v,w])</td>
<td>$x,y,z$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>5</td>
<td>$z,x,y$ ([w,u,v])</td>
<td>$z,x,y$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>6</td>
<td>$z,x,y$ ([w,u,v])</td>
<td>$z,x,y$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>7</td>
<td>$z,x,y$ ([w,u,v])</td>
<td>$z,x,y$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>8</td>
<td>$z,x,y$ ([w,u,v])</td>
<td>$z,x,y$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>9</td>
<td>$y,z,x$ ([v,w,u])</td>
<td>$y,z,x$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>10</td>
<td>$y,z,x$ ([v,w,u])</td>
<td>$y,z,x$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>11</td>
<td>$y,z,x$ ([v,w,u])</td>
<td>$y,z,x$</td>
<td>$1,0,0$</td>
</tr>
<tr>
<td>12</td>
<td>$y,z,x$ ([v,w,u])</td>
<td>$y,z,x$</td>
<td>$1,0,0$</td>
</tr>
</tbody>
</table>

Continued
| 6 | g | mm2.. | x,1/2,0 [0,0,0] | x,1/2,0 [0,0,0] | 0,x,1/2 [0,0,0] |
|   |   |        | 0,x,1/2 [0,0,0] | 1/2,0,x [0,0,0] | 1/2,0,x [0,0,0] |
| 6 | f | mm2.. | x,0,1/2 [0,0,0] | x,0,1/2 [0,0,0] | 1/2,x,0 [0,0,0] |
|   |   |        | 1/2,x,0 [0,0,0] | 0,1/2,x [0,0,0] | 0,1/2,x [0,0,0] |
| 6 | e | mm2.. | x,0,0 [0,0,0]   | x,0,0 [0,0,0]   | 0,x,0 [0,0,0]   |
|   |   |        | 0,x,0 [0,0,0]   | 0,0,x [0,0,0]   | 0,0,x [0,0,0]   |
| 3 | d | mmm.. | 1/2,0,0 [0,0,0] | 0,1/2,0 [0,0,0] | 0,0,1/2 [0,0,0] |
| 3 | c | mmm.. | 0,1/2,1/2 [0,0,0]| 1/2,0,1/2 [0,0,0]| 1/2,1/2,0 [0,0,0]|
| 1 | b | m\bar{3}.  | 1/2,1/2,1/2 [0,0,0]|                   |                  |
| 1 | a | m\bar{3}.  | 0,0,0 [0,0,0]   |                   |                  |

**Symmetry of Special Projections**

Along [0,0,1] p2mm1'

\[ \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \]

Origin at 0,0,z

Along [1,1,1] p6'

\[ \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \quad \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3 \]

Origin at x,x,x

Along [1,1,0] p2'\text{mm}'

\[ \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = (-\mathbf{a} + \mathbf{b})/2 \]

Origin at x,x,0
Origin at center (m$\overline{3}$1')

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min (x,y)$

Vertices

0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/2,1/2,1/2

Symmetry Operations

For $1^+ + set$

(1) 1
(1 | 0,0,0)

(2) $2 \ 0,0,z$
($2_z | 0,0,0$)

(3) $2 \ 0,y,0$
($2_y | 0,0,0$)

(4) $2 \ x,0,0$
($2_x | 0,0,0$)

(5) $3^+ x,x,x$
($3_{xyz} | 0,0,0$)

(6) $3^+ x,x,x$
($3_{xyz}^{-1} | 0,0,0$)

(7) $3^+ x,x,x$
($3_{xyz} | 0,0,0$)

(8) $3^+ x,x,x$
($3_{xyz}^{-1} | 0,0,0$)

(9) $3^+ x,x,x$
($3_{xyz}^{-1} | 0,0,0$)

(10) $3^+ x,x,x$
($3_{xyz} | 0,0,0$)

(11) $3^+ x,x,x$
($3_{xyz} | 0,0,0$)

(12) $3^+ x,x,x$
($3_{xyz}^{-1} | 0,0,0$)

Continued

200.2.1517

Pm$\overline{3}$1'
For 1' + set

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>1 + 1' +</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x, y, z [0, 0, 0]</td>
</tr>
<tr>
<td>2</td>
<td>x', y', z' [0, 0, 0]</td>
</tr>
<tr>
<td>3</td>
<td>x, y, z' [0, 0, 0]</td>
</tr>
<tr>
<td>4</td>
<td>x, y, z [0, 0, 0]</td>
</tr>
<tr>
<td>5</td>
<td>z, x, y [0, 0, 0]</td>
</tr>
<tr>
<td>6</td>
<td>z', x', y' [0, 0, 0]</td>
</tr>
<tr>
<td>7</td>
<td>z, x, y' [0, 0, 0]</td>
</tr>
<tr>
<td>8</td>
<td>z, x, y [0, 0, 0]</td>
</tr>
<tr>
<td>9</td>
<td>y, z, x [0, 0, 0]</td>
</tr>
<tr>
<td>10</td>
<td>y', z', x' [0, 0, 0]</td>
</tr>
<tr>
<td>11</td>
<td>y, z, x' [0, 0, 0]</td>
</tr>
<tr>
<td>12</td>
<td>y, z, x [0, 0, 0]</td>
</tr>
<tr>
<td>13</td>
<td>x, y, z [0, 0, 0]</td>
</tr>
<tr>
<td>14</td>
<td>x, y, z' [0, 0, 0]</td>
</tr>
<tr>
<td>15</td>
<td>x, y, z [0, 0, 0]</td>
</tr>
<tr>
<td>16</td>
<td>x, y, z [0, 0, 0]</td>
</tr>
<tr>
<td>17</td>
<td>z, x, y [0, 0, 0]</td>
</tr>
<tr>
<td>18</td>
<td>z', x', y' [0, 0, 0]</td>
</tr>
<tr>
<td>19</td>
<td>z, x, y [0, 0, 0]</td>
</tr>
<tr>
<td>20</td>
<td>z, x, y [0, 0, 0]</td>
</tr>
<tr>
<td>21</td>
<td>y, z, x [0, 0, 0]</td>
</tr>
<tr>
<td>22</td>
<td>y, z, x' [0, 0, 0]</td>
</tr>
<tr>
<td>23</td>
<td>y, z, x [0, 0, 0]</td>
</tr>
<tr>
<td>24</td>
<td>y, z, x [0, 0, 0]</td>
</tr>
</tbody>
</table>

Generators selected

(1); t(1, 0, 0); t(0, 1, 0); t(0, 0, 1); (2); (3); (5); (13); 1'.
Symmetry of Special Projections

Along [0, 0, 1] p2mm' 1'  
\( a^* = a \)  
\( b^* = b \)  
Origin at 0, 0, z

Along [1, 1, 1] p61'  
\( a^* = (2a - b - c)/3 \)  
\( b^* = (-a + 2b - c)/3 \)  
Origin at x, x, x

Along [1, 1, 0] p2mm' 1'  
\( a^* = (-a + b)/2 \)  
\( b^* = c \)  
Origin at x, x, 0

\( \text{Symmetry of Special Projections} \)

\( \text{Along [0, 0, 1]} \quad \text{p2mm' 1'} \)
\( a^* = a \quad b^* = b \)
Origin at 0, 0, z

\( \text{Along [1, 1, 1]} \quad \text{p61'} \)
\( a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \)
Origin at x, x, x

\( \text{Along [1, 1, 0]} \quad \text{p2mm' 1'} \)
\( a^* = (-a + b)/2 \quad b^* = c \)
Origin at x, x, 0

\( \text{Cubic} \)

200.3.1517  
Pm31'
Origin at center (m'3')

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min(x, y)\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2\]

Symmetry Operations

(1) 1
    (1 | 0,0,0)

(2) 2 0,0,z
    (2_z | 0,0,0)

(3) 2 0,y,0
    (2_y | 0,0,0)

(4) 2 x,0,0
    (2_z | 0,0,0)

(5) 3^+ x,x,x
    (3_{xyz} | 0,0,0)

(6) 3^+ \bar{x},x,\bar{x}
    (3_{xyz}^{-1} | 0,0,0)

(7) 3^+ x,x,\bar{x}
    (3_{xyz}^{-1} | 0,0,0)

(8) 3^+ \bar{x},x,\bar{x}
    (3_{xyz}^{-1} | 0,0,0)

(9) 3^- x,x,x
    (3_{xyz}^{-1} | 0,0,0)

(10) 3^- \bar{x},x,\bar{x}
    (3_{xyz} | 0,0,0)

(11) 3^- \bar{x},x,\bar{x}
    (3_{xyz} | 0,0,0)

(12) 3^- x,x,\bar{x}
    (3_{xyz} | 0,0,0)

Continued
(13) 1 0,0,0
   (1) 0,0,0)
(14) m' x,y,0
   (m, [0,0,0])
(15) m' x,0,z
   (m, [0,0,0])
(16) m' 0,0,z
   (m, [0,0,0])

(17) y' x' x' x, x; 0,0,0
   (x, y, x; 0,0,0)
(18) 3' x' x' x; 0,0,0
   (3' x, y, x; 0,0,0)
(19) 3' x' x, x; 0,0,0
   (3' x, y, x; 0,0,0)
(20) 3' x' x, x; 0,0,0
   (3' x, y, x; 0,0,0)

(21) 3' x' x, x; 0,0,0
   (3' x, y, x; 0,0,0)
(22) 3' x' x, x; 0,0,0
   (3' x, y, x; 0,0,0)
(23) 3' x' x, x; 0,0,0
   (3' x, y, x; 0,0,0)
(24) 3' x' x, x; 0,0,0
   (3' x, y, x; 0,0,0)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

24  l  1

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) x,y,z [u,v,w]
(4) x,y,z [u,v,w]
(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]
(9) y,z,x [v,w,u]
(10) y,z,x [v,w,u]
(11) y,z,x [v,w,u]
(12) y,z,x [v,w,u]
(13) x,y,z [u,v,w]
(14) x,y,z [u,v,w]
(15) x,y,z [u,v,w]
(16) x,y,z [u,v,w]
(17) x,y,z [u,v,w]
(18) x,y,z [u,v,w]
(19) x,y,z [u,v,w]
(20) x,y,z [u,v,w]
(21) x,y,z [v,w,u]
(22) y,z,x [v,w,u]
(23) y,z,x [v,w,u]
(24) y,z,x [v,w,u]

12  k  m'..  1/2,y,z [0,v,w]
   1/2,y,z [0,v,w]
   1/2,y,z [0,v,w]
   1/2,y,z [0,v,w]
   z,1/2,y [w,0,v]
   z,1/2,y [w,0,v]
   z,1/2,y [w,0,v]
   z,1/2,y [w,0,v]
   y,z,1/2 [v,w,0]
   y,z,1/2 [v,w,0]
   y,z,1/2 [v,w,0]
   y,z,1/2 [v,w,0]

12  j  m'..  0,y,z [0,v,w]
   0,y,z [0,v,w]
   0,y,z [0,v,w]
   0,y,z [0,v,w]
   z,0,y [w,0,v]
   z,0,y [w,0,v]
   z,0,y [w,0,v]
   z,0,y [w,0,v]
   y,z,0 [v,w,0]
   y,z,0 [v,w,0]
   y,z,0 [v,w,0]
   y,z,0 [v,w,0]

8  i  .3.  x,x,x [u,u,u]
   x,x,x [u,u,u]
   x,x,x [u,u,u]
   x,x,x [u,u,u]
   x,x,x [u,u,u]
   x,x,x [u,u,u]
   x,x,x [u,u,u]

6  h  m'm'2.. x,1/2,1/2 [u,0,0]
   x,1/2,1/2 [u,0,0]
   x,1/2,1/2 [u,0,0]
   x,1/2,1/2 [u,0,0]
   x,1/2,1/2 [u,0,0]
   x,1/2,1/2 [u,0,0]
   x,1/2,1/2 [u,0,0]

Continued  200.3.1518  Pm'3'

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6 g m'm'2. x,1/2,0 [u,0,0]  $\bar{x},1/2,0$ [u,0,0]  0,x,1/2 [u,0,0]
   0,x,1/2 [u,0,0]  1/2,0,x [0,0,u]  1/2,0,x [0,0,u]
6 f m'm'2. x,0,1/2 [u,0,0]  $\bar{x},0,1/2$ [u,0,0]  1/2,x,0 [u,0,0]
   1/2,x,0 [u,0,0]  0,1/2,x [0,0,u]  0,1/2,x [0,0,u]
6 e m'm'2. x,0,0 [u,0,0]  $x,0,0$ [u,0,0]  0,x,0 [u,0,0]
   0,x,0 [u,0,0]  0,0,x [0,0,u]  0,0,x [0,0,u]
3 d m'm'm'.. 1/2,0,0 [0,0,0]  0,1/2,0 [0,0,0]  0,0,1/2 [0,0,0]
3 c m'm'm'.. 0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]
1 b m'3. 1/2,1/2,1/2 [0,0,0]
1 a m'3. 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p2m1m'  
$\mathbf{a}^{*} = \mathbf{a}  \quad \mathbf{b}^{*} = \mathbf{b}$  
Origin at 0,0,z

Along [1,1,1] p6  
$\mathbf{a}^{*} = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3  \quad \mathbf{b}^{*} = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3$  
Origin at x,x,x

Along [1,1,0] p2m1m'  
$\mathbf{a}^{*} = (\mathbf{a} + \mathbf{b})/2  \quad \mathbf{b}^{*} = \mathbf{c}$  
Origin at x,x,0
**Origin** at center (m\(\overline{3}\))

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \text{min}(x, y)\]

**Vertices**

\[0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2\]

**Symmetry Operations**

For \((0,0,0)\) + set

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 3^{+} x,x,x \\
(3) & \quad 3^{+} x,x,x \\
(4) & \quad 3^{+} x,x,x \\
(5) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(7) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(8) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(9) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(10) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^{+} x,x,x \quad (3_{xyz}|0,0,0) \\
(13) & \quad 1 \quad 0,0,0 \\
(14) & \quad m \quad x,y,0 \\
(15) & \quad m \quad x,0,z \\
(16) & \quad m \quad 0,y,z \\
(17) & \quad x,x,x; 0,0,0 \\
(18) & \quad 3^{+} x,x,x; 0,0,0 \\
(19) & \quad 3^{+} x,x,x; 0,0,0 \\
(20) & \quad 3^{+} x,x,x; 0,0,0 \\
(21) & \quad 3^{+} x,x,x; 0,0,0 \\
(22) & \quad 3^{+} x,x,x; 0,0,0 \\
(23) & \quad 3^{+} x,x,x; 0,0,0 \\
(24) & \quad 3^{+} x,x,x; 0,0,0
\end{align*}

For \((1,0,0)\)' + set

\begin{align*}
(1) & \quad t'(1,0,0) \\
(2) & \quad 2' 1/2,0,z \\
(3) & \quad 2' 1/2,0,z \\
(4) & \quad 2' -1/2,1/2 \\
(5) & \quad x+2/3, x-1/2, 1/3 \\
(6) & \quad (3_{xyz}|1,0,0) \\
(7) & \quad (3_{xyz}|1,0,0) \\
(8) & \quad (3_{xyz}|1,0,0) \\
(9) & \quad x+1/3, x+1/3, x \\
(10) & \quad (3_{xyz}|1,0,0) \\
(11) & \quad (3_{xyz}|1,0,0) \\
(12) & \quad (3_{xyz}|1,0,0) \\
(13) & \quad 1\overline{1} 2/0,0 \\
(14) & \quad a'(1,0,0) \\
(15) & \quad a'(1,0,0) \\
(16) & \quad m' 1/2, y,z \\
(17) & \quad x+1, x+1, x \\
(18) & \quad (3_{xyz}|1,0,0) \\
(19) & \quad (3_{xyz}|1,0,0) \\
(20) & \quad (3_{xyz}|1,0,0) \\
(21) & \quad x+1, x+1, x \\
(22) & \quad (3_{xyz}|1,0,0) \\
(23) & \quad (3_{xyz}|1,0,0) \\
(24) & \quad (3_{xyz}|1,0,0)
\end{align*}
**Generators selected**

(1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13).

<table>
<thead>
<tr>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
</tr>
<tr>
<td>48 l 1</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
</tr>
<tr>
<td>(13) x, ̅y, ̅z [u,v,w]</td>
</tr>
<tr>
<td>(17) ̅z,x, ̅y [w,u,v]</td>
</tr>
<tr>
<td>(21) ̅y,z,x [v,w,u]</td>
</tr>
</tbody>
</table>

| 24 k m'.. | 1/2,y,z [0,v,w] | 1/2,y, ̅z [0, ̅v,w] | 1/2,y, ̅z [0, ̅v,w] |
| 24 j m.. | 0,y,z [u,0,0] | 0,y, ̅z [u,0,0] | 0,y, ̅z [u,0,0] |
| 16 i .3: | x,x,x [u,u,u] | x, ̅x,x [u, ̅u,u] | x, ̅x,x [u, ̅u,u] |
| 12 h m'm2.. | x,1/2,1/2 [u,0,0] | x,1/2,1/2 [u,0,0] | 1/2,x,1/2 [0,u,0] |
| 12 g m'm2'.. | x,1/2,0 [0,0,w] | x, ̅1/2,0 [0, ̅0,w] | 0,x,1/2 [w,0,0] |
| 12 f mm'2'.. | x,0,1/2 [0,v,0] | x,0, ̅1/2 [0, ̅v,0] | 1/2,x,0 [0,0,v] |
| 12 e mm2.. | x,0,0 [0,0,0] | x,0, ̅0 [0, ̅0,0] | 0,x,0 [0,0,0] |

200.4.1519 - 3 - 3366
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Symmetry</th>
<th>0,0,0 [0,0,0]</th>
<th>1/2,1,2 [0,0,0]</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p2mm1'</td>
<td>a* = a, b* = b</td>
<td>a* = (2a - b - c)/3</td>
<td>Origin at 0,0,z</td>
</tr>
<tr>
<td>Along [1,1,1]</td>
<td>p61'</td>
<td>a* = (2a - b - c)/3, b* = (-a + 2b - c)/3</td>
<td>Origin at x,x,x</td>
<td></td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p122</td>
<td>a* = (a - b + c)/3, b* = c</td>
<td>Origin at x-1/4,x+1/4,0</td>
<td></td>
</tr>
</tbody>
</table>

Continued

6 d m'mm.. 1/2,0,0 [0,0,0] 0,1/2,0 [0,0,0] 0,0,1/2 [0,0,0]
6 c mmm.. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]
2 b m'3: 1/2,1/2,1/2 [0,0,0]
2 a m'3': 0,0,0 [0,0,0]
Pn$\bar{3}$

201.1.1520

$\bar{m}$3

P2/n3

Cubic

Origin at 23, at $-1/4,-1/4,-1/4$ from center (3)

Asymmetric unit

$0 \leq x \leq 1$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$; $y \leq \min (x,1-x)$; $z \leq y$

Vertices

$0,0,0$ $1,0,0$ $1/2,1/2,0$ $1/2,1/2,1/2$

Symmetry Operations

(1) 1
(2) $0,0,z$ $(2_z|0,0,0)$
(3) $0,y,0$ $(2_y|0,0,0)$
(4) $x,0,0$ $(2_x|0,0,0)$
(5) $3^+ x,x,x$ $(3_{xyz}|0,0,0)$
(6) $3^- x,x,x$ $(3_{xyz}^{-1}|0,0,0)$
(7) $3^+ x,x,x$ $(3_{xyz}|0,0,0)$
(8) $3^- x,x,x$ $(3_{xyz}^{-1}|0,0,0)$
(9) $3^+ x,x,x$ $(3_{xyz}|0,0,0)$
(10) $3^- x,x,x$ $(3_{xyz}^{-1}|0,0,0)$
(11) $3^+ x,x,x$ $(3_{xyz}|0,0,0)$
(12) $3^- x,x,x$ $(3_{xyz}^{-1}|0,0,0)$
Continued

(13) $\overline{1} 1/4,1/4,1/4$
(14) $n (1/2,1/2,0)$ $x,y,1/4$
(15) $n (1/2,0,1/2)$ $x,1/4,z$
(16) $n (0,1/2,1/2)$ $1/4,y,z$

(17) $3^+ x,x,x$
(18) $3^+ x+1/4,1/4,1/4$
(19) $3^+ x+1/4,1/4,3/4$
(20) $3^+ x+1,1,1$

(21) $3^+ x,x,x$
(22) $3^+ x+1,1,1$
(23) $3^+ x,x+1,1$
(24) $3^+ x+1,x,x$

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

24 h 1

(1) $x,y,z [u,v,w]$
(2) $x,y,z [u,v,w]$
(3) $x,y,z [u,v,w]$
(4) $x,y,z [u,v,w]$
(5) $z,x,y [w,u,v]$
(6) $z,x,y [w,u,v]$
(7) $z,x,y [w,u,v]$
(8) $z,x,y [w,u,v]$
(9) $y,z,x [v,w,u]$
(10) $y,z,x [v,w,u]$
(11) $y,z,x [v,w,u]$
(12) $y,z,x [v,w,u]$

(13) $x+1/2,y+1/2,z+1/2 [u,v,w]$
(14) $x+1/2,y+1/2,z+1/2 [u,v,w]$
(15) $x+1/2,y+1/2,z+1/2 [u,v,w]$
(16) $x+1/2,y+1/2,z+1/2 [u,v,w]$
(17) $x+1/2,x+1/2,y+1/2 [w,u,v]$
(18) $x+1/2,x+1/2,y+1/2 [w,u,v]$
(19) $x+1/2,x+1/2,y+1/2 [w,u,v]$
(20) $x+1/2,x+1/2,y+1/2 [w,u,v]$
(21) $y+1/2,z+1/2,x+1/2 [v,w,u]$
(22) $y+1/2,z+1/2,x+1/2 [v,w,u]$
(23) $y+1/2,z+1/2,x+1/2 [v,w,u]$
(24) $y+1/2,z+1/2,x+1/2 [v,w,u]$

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Continued

| 6 | d | 222. | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] |
|   |   |       | 1/2,0,0 [0,0,0] | 0,1/2,0 [0,0,0] | 0,0,1/2 [0,0,0] |
| 4 | c | $\overline{3}$. | 3/4,3/4,3/4 [u,u,u] | 1/4,1/4,3/4 [u,u,u] | 1/4,3/4,1/4 [u,u,u] | 3/4,1/4,1/4 [u,u,u] |
| 4 | b | $\overline{3}$. | 1/4,1/4,1/4 [u,u,u] | 3/4,3/4,1/4 [u,u,u] | 3/4,1/4,3/4 [u,u,u] | 1/4,3/4,3/4 [u,u,u] |
| 2 | a | 23. | 0,0,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

**Symmetry of Special Projections**

Along $[0,0,1]$  \( c_{2} \) 2$m'$m'  
\( a^{*} = a \) \( b^{*} = b \)  
Origin at 0,0,z

Along $[1,1,1]$  \( p6' \)  
\( a^{*} = (2a - b - c)/3 \) \( b^{*} = (a + 2b - c)/3 \)  
Origin at x,x,x

Along $[1,1,0]$  \( p2'm'm' \)  
\( a^{*} = c \) \( b^{*} = (-a + b)/2 \)  
Origin at x,x,1/4

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Origin at 231', at -1/4,-1/4,-1/4 from center (31')

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min (x,1-x); \quad z \leq y \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1,0,0 & \quad 1/2,1/2,0 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & & (2) & & (3) & & (4) \\
1 & & 2 & & 0,0,z & & 0 \quad 0,0,0 & & 2_x \quad 0,0,0 & & 2 \quad x,0,0 & & 2 \quad x,0,0,0 \\
(1 | 0,0,0) & & (2_z | 0,0,0) & & (2_y | 0,0,0) & & (2_z | 0,0,0) \\
(5) & & (6) & & (7) & & (8) \\
3^+ & & 3^+ & & 3^+ & & 3^+
\quad x,x,x & \quad x,x,x & \quad x,x,x & \quad x,x,x
\quad (3_{xyz} | 0,0,0) & \quad (3_{xyz}^{-1} | 0,0,0) & \quad (3_{xyz} | 0,0,0) & \quad (3_{xyz}^{-1} | 0,0,0) \\
(9) & & (10) & & (11) & & (12) \\
3^+ & & 3^+ & & 3^+ & & 3^+
\quad x,x,x & \quad x,x,x & \quad x,x,x & \quad x,x,x
\quad (3_{xyz}^{-1} | 0,0,0) & \quad (3_{xyz} | 0,0,0) & \quad (3_{xyz}^{-1} | 0,0,0) & \quad (3_{xyz} | 0,0,0)
\end{align*}
\]

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(13) $\overline{1}$ 1/4,1/4,1/4
(1 | 1/2,1/2,1/2)

(14) n (1/2,1/2,0) x,y,1/4
(m' | 1/2,1/2,1/2)

(15) n (1/2,0,1/2) x,1/4,z
(m' | 1/2,1/2,1/2)

(16) n (0,1/2,1/2) 1/4,y,z
(m' | 1/2,1/2,1/2)

(17) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

(18) $\overline{3}'$ x-1,x+1,x;
-1/4,1/4,3/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

(19) $\overline{3}'$ x,x+1,x;
1/4,3/4,-1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

(20) $\overline{3}'$ x+1,x,x;
3/4,-1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

(21) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

(22) $\overline{3}'$ x+1,x-1,x;
1/4,-1/4,3/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

(23) $\overline{3}'$ x,x+1,x;
-1/4,3/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

(24) $\overline{3}'$ x+1,x,x;
3/4,1/4,-1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)

---

**For 1' + set**

(1) 1'
(1 | 0,0,0)'

(2) 2' 0,0,z
(2z | 0,0,0)'

(3) 2' y,0
(2y | 0,0,0)'

(4) 2' x,0,0
(2x | 0,0,0)'

(5) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(6) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(7) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(8) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(9) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(10) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(11) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(12) $\overline{3}'$ x,x,x
($\overline{3}_{xyz}$ | 0,0,0)'

(13) $\overline{1}'$ 1/4,1/4,1/4
($\overline{1}$ | 1/2,1/2,1/2)'

(14) n' (1/2,1/2,0) x,y,1/4
(m' | 1/2,1/2,1/2)'

(15) n' (1/2,0,1/2) x,1/4,z
(m' | 1/2,1/2,1/2)'

(16) n' (0,1/2,1/2) 1/4,y,z
(m' | 1/2,1/2,1/2)'

(17) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

(18) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

(19) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

(20) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

(21) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

(22) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

(23) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

(24) $\overline{3}'$ x,x,x;
1/4,1/4,1/4
($\overline{3}_{xyz}$ | 1/2,1/2,1/2)'

---

**Generators selected**
(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

24 h 11'

(1) x,y,z [0,0,0]
(2) x,y,z [0,0,0]
(3) x,y,z [0,0,0]
(4) x,y,z [0,0,0]

(5) z,x,y [0,0,0]
(6) z,x,y [0,0,0]
(7) z,x,y [0,0,0]
(8) z,x,y [0,0,0]

(9) y,z,x [0,0,0]
(10) y,z,x [0,0,0]
(11) y,z,x [0,0,0]
(12) y,z,x [0,0,0]

(13) x+1/2,y+1/2,z+1/2 [0,0,0]
(14) x+1/2,y+1/2,z+1/2 [0,0,0]
(15) x+1/2,y+1/2,z+1/2 [0,0,0]
(16) x+1/2,y+1/2,z+1/2 [0,0,0]

(17) z+1/2,x+1/2,y+1/2 [0,0,0]
(18) z+1/2,x+1/2,y+1/2 [0,0,0]
(19) z+1/2,x+1/2,y+1/2 [0,0,0]
(20) z+1/2,x+1/2,y+1/2 [0,0,0]

(21) y+1/2,z+1/2,x+1/2 [0,0,0]
(22) y+1/2,z+1/2,x+1/2 [0,0,0]
(23) y+1/2,z+1/2,x+1/2 [0,0,0]
(24) y+1/2,z+1/2,x+1/2 [0,0,0]
<table>
<thead>
<tr>
<th>12</th>
<th>g</th>
<th>2\cdot1'</th>
<th>x,1/2,0 [0,0,0]</th>
<th>$\overline{x},1/2,0 [0,0,0]$</th>
<th>0,x,1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,x,1/2 [0,0,0]</td>
<td>$1/2,0,x [0,0,0]$</td>
<td>$1/2,0,\overline{x} [0,0,0]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$x+1/2,0,1/2$ [0,0,0]</td>
<td>$x+1/2,0,1/2$ [0,0,0]</td>
<td>$1/2,x+1/2,0$ [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$1/2,x+1/2,0$ [0,0,0]</td>
<td>$0,1/2,\overline{x}+1/2$ [0,0,0]</td>
<td>$0,1/2,x+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>12</td>
<td>f</td>
<td>2\cdot1'</td>
<td>x,0,0 [0,0,0]</td>
<td>$\overline{x},0,0 [0,0,0]$</td>
<td>0,x,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0,\overline{x},0 [0,0,0]</td>
<td>0,0,x [0,0,0]</td>
<td>0,0,\overline{x} [0,0,0]</td>
</tr>
<tr>
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<td></td>
<td>$x+1/2,1/2,1/2$ [0,0,0]</td>
<td>$x+1/2,1/2,1/2$ [0,0,0]</td>
<td>$1/2,x+1/2,1/2$ [0,0,0]</td>
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<td>$1/2,x+1/2,1/2$ [0,0,0]</td>
<td>$1/2,1/2,\overline{x}+1/2$ [0,0,0]</td>
<td>$1/2,1/2,x+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>e</td>
<td>.3.1'</td>
<td>x,x,x [0,0,0]</td>
<td>$\overline{x},\overline{x},\overline{x}$ [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$x,x,\overline{x}$ [0,0,0]</td>
<td>$x,\overline{x},\overline{x}$ [0,0,0]</td>
<td>$\overline{x},\overline{x},x$ [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>$x+1/2,\overline{x}+1/2,\overline{x}+1/2$ [0,0,0]</td>
<td>$x+1/2,\overline{x}+1/2,\overline{x}+1/2$ [0,0,0]</td>
<td>$1/2,\overline{x}+1/2,\overline{x}+1/2$ [0,0,0]</td>
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<td>$x+1/2,\overline{x}+1/2,\overline{x}+1/2$ [0,0,0]</td>
<td>$\overline{x}+1/2,\overline{x}+1/2,\overline{x}+1/2$ [0,0,0]</td>
<td>$\overline{x}+1/2,\overline{x}+1/2,\overline{x}+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>d</td>
<td>222..1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>$1/2,0,1/2$ [0,0,0]</td>
<td>$1/2,1/2,0$ [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$1/2,0,0$ [0,0,0]</td>
<td>$1/2,0,0$ [0,0,0]</td>
<td>$0,1/2,0$ [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>.\overline{3}.1'</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
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<td></td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
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<tr>
<td>4</td>
<td>b</td>
<td>.\overline{3}.1'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>23.1'</td>
<td>0,0,0 [0,0,0]</td>
<td>$1/2,1/2,1/2$ [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1] c2mm1'**
  - $a^* = a$  
  - $b^* = b$

- **Along [1,1,1] p61'**
  - $a^* = (2a - b - c)/3$  
  - $b^* = -(a + 2b - c)/3$

- **Along [1,1,0] p2mm1'**
  - $a^* = (a + b)/2$  
  - $b^* = c$

**Origin**

- Origin at 0,0,0 for $c2mm1'$
- Origin at x,x,x for $p61'$
- Origin at x,x,1/4 for $p2mm1'$
Origin at 23, at -1/4,-1/4,-1/4 from center (3'')

Asymmetric unit

0 ≤ x ≤ 1; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ min (x,1-x); z ≤ y

Vertices 0,0,0 1,0,0 1/2,1/2,0 1/2,1/2,1/2

Symmetry Operations

(1) 1
   (1|0,0,0)

(2) 2 0,0,z
    (2z|0,0,0)

(3) 2 0,y,0
    (2y|0,0,0)

(4) 2 x,0,0
    (2z|0,0,0)

(5) 3' x,x,x
    (3xyz|0,0,0)

(6) 3' x,x,x
    (3xyz|0,0,0)

(7) 3' x, x, x
    (3xyz|0,0,0)

(8) 3' x,x,x
    (3xyz|0,0,0)

(9) 3' x,x,x
    (3xyz'1|0,0,0)

(10) 3' x,x,x
     (3xyz'1|0,0,0)

(11) 3' x,x,x
     (3xyz|0,0,0)

(12) 3' x,x,x
     (3xyz|0,0,0)
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 h 1

(1) x,y,z [u,v,w] (2) x, y, z [u, v, w] (3) x, y, z [u, v, w] (4) x, y, z [u, v, w]

(5) z,x,y [w,u,v] (6) z, x, y [w, u, v] (7) z, x, y [w, u, v] (8) z, x, y [w, u, v]

(9) y,z,x [v,w,u] (10) y, z, x [v, w, u] (11) y, z, x [v, w, u] (12) y, z, x [v, w, u]

(13) x+1/2, y+1/2, z+1/2 [u, v, w] (14) x+1/2, y+1/2, z+1/2 [u, v, w] (15) x+1/2, y+1/2, z+1/2 [u, v, w] (16) x+1/2, y+1/2, z+1/2 [u, v, w]

(17) z+1/2, y+1/2, x+1/2 [w, u, v] (18) z+1/2, y+1/2, x+1/2 [w, u, v] (19) z+1/2, y+1/2, x+1/2 [w, u, v] (20) z+1/2, x+1/2, y+1/2 [w, u, v]

(21) y+1/2, z+1/2, x+1/2 [v, w, u] (22) y+1/2, z+1/2, x+1/2 [v, w, u] (23) y+1/2, z+1/2, x+1/2 [v, w, u] (24) y+1/2, z+1/2, x+1/2 [v, w, u]

12 g 2.. x,1/2,0 [u,0,0] x,1/2,0 [u,0,0] 0,x,1/2 [0,u,0]

0,x,1/2 [0,u,0] 1/2,0,x [0,0,u] 1/2,0,x [0,0,u]

x+1/2,0,1/2 [u,0,0] x+1/2,0,1/2 [u,0,0] 1/2,x+1/2,0 [0,u,0]

1/2,x+1/2,0 [0,u,0] 0,1/2,x+1/2 [0,0,u] 0,1/2,x+1/2 [0,0,u]

12 f 2.. x,0,0 [u,0,0] x,0,0 [u,0,0] 0,x,0 [0,u,0]

0,x,0 [0,u,0] 0,x,0 [0,u,0] 0,0,x [0,0,u]

x+1/2,1/2,1/2 [u,0,0] x+1/2,1/2,1/2 [u,0,0] 1/2,x+1/2,1/2 [0,u,0]

1/2,x+1/2,1/2 [0,u,0] 1/2,1/2,x+1/2 [0,0,u] 1/2,1/2,x+1/2 [0,0,u]

8 e .3. x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]

x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]
<table>
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<th>222..</th>
<th>0,1/2, 1/2 [0,0,0]</th>
<th>1/2,0, 1/2 [0,0,0]</th>
<th>1/2,1/2,0 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>.3'</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
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<td>1/4,3/4,3/4 [0,0,0]</td>
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<td></td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>.3'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
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<td>1/4,3/4,3/4 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>23.</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**  c2m'm'
  - \( a^* = a \) \( b^* = b \)
  - Origin at 0,0,z

- **Along [1,1,1]**  p6
  - \( a^* = (2a - b - c)/3 \) \( b^* = (-a + 2b - c)/3 \)
  - Origin at x,x,x

- **Along [1,1,0]**  p2m'm'
  - \( a^* = (-a + b)/2 \) \( b^* = c \)
  - Origin at x,x,1/4
Origin at 23, at -1/4,-1/4,-1/4 from center (3)

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min(x,1-x); \quad z \leq y \]

Vertices

\( 0,0,0 \quad 1,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2 \)

Symmetry Operations

For \((0,0,0)\) + set

(1) \( 1 \)
(2) \( 2 \quad 0,0,z \)
(3) \( 2 \quad y,0 \)
(4) \( 2 \quad x,0,0 \)
(5) \( 3^+ \quad x,x,x \)
(6) \( 3^+ \quad x,x,x \)
(7) \( 3^+ \quad x,x,x \)
(8) \( 3^+ \quad x,x,x \)
(9) \( 3^- \quad x,x,x \)
(10) \( 3^- \quad x,x,x \)
(11) \( 3^- \quad x,x,x \)
(12) \( 3^- \quad x,x,x \)
(13) \( \overline{1} \quad 1/4,1/4,1/4 \)
(14) \( n \quad 1/2,1/2,0 \quad x,y,1/4 \)
(15) \( n \quad 1/2,0,1/2 \quad x,1/4,z \)
(16) \( n \quad 0,1/2,1/2 \quad 1/4,y,z \)
(17) \( \overline{3}^+ \quad x,x,x; \)
(18) \( \overline{3}^+ \quad x,x,x; \)
(19) \( \overline{3}^+ \quad x,x,x; \)
(20) \( \overline{3}^+ \quad x,x,x; \)
(21) \( \overline{3}^- \quad x,x,x; \)
(22) \( \overline{3}^- \quad x,x,x; \)
(23) \( \overline{3}^- \quad x,x,x; \)
(24) \( \overline{3}^- \quad x,x,x; \)

For \((1,0,0)\) + set

(1) \( t' \quad (1,0,0) \)
(2) \( 2' \quad 1/2,0,z \)
(3) \( 2' \quad 1/2,0,0 \)
(4) \( 2' \quad 1,0,0 \)
(5) \( 3'^+ \quad (1/3,1/3,1/3) \)
(6) \( 3'^+ \quad (1/3,1/3,1/3) \)
(7) \( 3'^+ \quad (1/3,1/3,1/3) \)
(8) \( 3'^+ \quad (1/3,1/3,1/3) \)
(9) \( 3'^- \quad (1/3,1/3,1/3) \)
(10) \( 3'^- \quad (1/3,1/3,1/3) \)
(11) \( 3'^- \quad (1/3,1/3,1/3) \)
(12) \( 3'^- \quad (1/3,1/3,1/3) \)
(13) \( \overline{1} \quad 3/4,1/4,1/4 \)
(14) \( n' \quad 3/2,1/2,0 \quad x,y,1/4 \)
(15) \( n' \quad 3/2,0,1/2 \quad x,1/4,z \)
(16) \( n' \quad 0,1/2,1/2 \quad 3/4,y,z \)
(17) \( \overline{3}^+ \quad x,x,x; \)
(18) \( \overline{3}^+ \quad x,x,x; \)
(19) \( \overline{3}^+ \quad x,x,x; \)
(20) \( \overline{3}^+ \quad x,x,x; \)
(21) \( \overline{3}^- \quad x,x,x; \)
(22) \( \overline{3}^- \quad x,x,x; \)
(23) \( \overline{3}^- \quad x,x,x; \)
(24) \( \overline{3}^- \quad x,x,x; \)

Generators selected

(1); \( t'(1,0,0); t'(0,0,1); \) (2); (3); (5); (13).
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<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>48 h 1</td>
<td></td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) z,x,y [w,u,v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) y,z,x [v,w,u]</td>
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<td>(13) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
<td>(14) x+1/2,y+1/2,z+1/2 [u,v,w]</td>
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<td>(17) z+1/2,x+1/2,y+1/2 [w,u,v]</td>
<td>(18) z+1/2,x+1/2,y+1/2 [w,u,v]</td>
</tr>
<tr>
<td>(21) y+1/2,z+1/2,x+1/2 [v,w,u]</td>
<td>(22) y+1/2,z+1/2,x+1/2 [v,w,u]</td>
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<tr>
<td>24 g 2'..</td>
<td>x,1/2,0 [v,w]</td>
</tr>
<tr>
<td>0,x,1/2 [w,0,v]</td>
<td>1/2,0,x [v,w,0]</td>
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<tr>
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<td>1/2,x+1/2,0 [w,0,v]</td>
<td>0,1/2,x+1/2 [v,w,0]</td>
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<tr>
<td>24 f 2..</td>
<td>x,0,0 [u,0,0]</td>
</tr>
<tr>
<td>0,x,0 [u,0,0]</td>
<td>0,0,x [0,u,0]</td>
</tr>
<tr>
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<td>x+1/2,1/2,1/2 [u,0,0]</td>
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<tr>
<td>1/2,x+1/2,1/2 [0,u,0]</td>
<td>1/2,1/2,x+1/2 [0,u,0]</td>
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<tr>
<td>16 e .3.</td>
<td>x,x,x [u,u,u]</td>
</tr>
<tr>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
</tr>
<tr>
<td>x+1/2,x+1/2,x+1/2 [u,u,u]</td>
<td>x+1/2,x+1/2,x+1/2 [u,u,u]</td>
</tr>
<tr>
<td>x+1/2,x+1/2,x+1/2 [u,u,u]</td>
<td>x+1/2,x+1/2,x+1/2 [u,u,u]</td>
</tr>
<tr>
<td>12 d 22'...</td>
<td>0,1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>1/2,0,0 [u,0,0]</td>
<td>1/2,0,0 [u,0,0]</td>
</tr>
<tr>
<td>0,1/2,0 [0,u,0]</td>
<td>0,1/2,0 [0,u,0]</td>
</tr>
<tr>
<td>4 c .3'.</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b .3.</td>
<td>1/4,1/4,1/4 [u,u,u]</td>
</tr>
<tr>
<td>3/4,3/4,1/4 [u,u,u]</td>
<td>3/4,1/4,3/4 [u,u,u]</td>
</tr>
<tr>
<td>2 a 23.</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Symmetry</th>
<th>a* = a</th>
<th>b* = b</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>c2mm1'</td>
<td></td>
<td></td>
<td>0,0,z</td>
</tr>
<tr>
<td>[1,1,1]</td>
<td>p61'</td>
<td>a* = (2a - b - c)/3</td>
<td>b* = (-a + 2b - c)/3</td>
<td>x,x,x</td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>p_c2mm</td>
<td>a* = (-a + b)/2</td>
<td>b* = c</td>
<td>x-1/4,x+1/4,1/4</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,x,x

Origin at x-1/4,x+1/4,1/4
Origin at center (m\textoverline{3})

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq \min(1/2-x,y)\)

Vertices \(0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4\)

Symmetry Operations

For \((0,0,0) + \) set

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2) & \quad (2_z|0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(3) & \quad (2_y|0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(4) & \quad (2_x|0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
(6) & \quad (3_{xyz}|0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
(7) & \quad (3_{xyz}^{-1}|0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
(8) & \quad (3_{xyz}^{-1}|0,0,0) \\
(9) & \quad 3^+ \quad x,x,x \\
(9) & \quad (3_{xyz}|0,0,0) \\
(10) & \quad 3^+ \quad x,x,x \\
(10) & \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^+ \quad x,x,x \\
(11) & \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^+ \quad x,x,x \\
(12) & \quad (3_{xyz}|0,0,0) \\
\end{align*}

Continued

\begin{align*}
(3) & \quad 2 \quad 0,0,z \\
(2) & \quad (2_z|0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(3) & \quad (2_y|0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(4) & \quad (2_x|0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
(6) & \quad (3_{xyz}^{-1}|0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
(7) & \quad (3_{xyz}^{-1}|0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
(8) & \quad (3_{xyz}^{-1}|0,0,0) \\
(9) & \quad 3^+ \quad x,x,x \\
(9) & \quad (3_{xyz}|0,0,0) \\
(10) & \quad 3^+ \quad x,x,x \\
(10) & \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^+ \quad x,x,x \\
(11) & \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^+ \quad x,x,x \\
(12) & \quad (3_{xyz}|0,0,0) \\
\end{align*}

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2) & \quad (2_z|0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(3) & \quad (2_y|0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(4) & \quad (2_x|0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
(6) & \quad (3_{xyz}^{-1}|0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
(7) & \quad (3_{xyz}^{-1}|0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
(8) & \quad (3_{xyz}^{-1}|0,0,0) \\
(9) & \quad 3^+ \quad x,x,x \\
(9) & \quad (3_{xyz}|0,0,0) \\
(10) & \quad 3^+ \quad x,x,x \\
(10) & \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^+ \quad x,x,x \\
(11) & \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^+ \quad x,x,x \\
(12) & \quad (3_{xyz}^{-1}|0,0,0) \\
\end{align*}

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2) & \quad (2_z|0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(3) & \quad (2_y|0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(4) & \quad (2_x|0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
(6) & \quad (3_{xyz}^{-1}|0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
(7) & \quad (3_{xyz}^{-1}|0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
(8) & \quad (3_{xyz}^{-1}|0,0,0) \\
(9) & \quad 3^+ \quad x,x,x \\
(9) & \quad (3_{xyz}|0,0,0) \\
(10) & \quad 3^+ \quad x,x,x \\
(10) & \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^+ \quad x,x,x \\
(11) & \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^+ \quad x,x,x \\
(12) & \quad (3_{xyz}^{-1}|0,0,0) \\
\end{align*}

Continued
(13) $\bar{1}$, 0,0,0  
     (1, 0,0,0)  

(14) $m$, x,y,0  
     (m, 0,0,0)  

(15) $m$, x,0,z  
     (m, 0,0,0)  

(16) $m$, 0,y,z  
     (m, 0,0,0)  

(17) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

(18) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

(19) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

(20) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

(21) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

(22) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

(23) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

(24) $\bar{3}$, x,x,x; 0,0,0  
     (3, 0,0,0)  

For (0,1/2,1/2) + set

(1) $t$, 0,1/2,1/2  
     (1, 0,1/2,1/2)  

(2) 2, 0,0,1/2  
     (2, 0,1/2,1/2)  

(3) 2, 0,1/2,0  
     (2, 0,1/2,1/2)  

(4) 2, 0,1/2,1/2  
     (2, 0,1/2,1/2)  

(5) $3$, (1/3,1/3,1/3)  
     x-1/3,x-1/3,x  
     (3, 0,1/2,1/2)  

(6) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(7) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(8) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

For (1/2,0,1/2) + set

(1) $t$, 1/2,0,1/2  
     (1, 1/2,0,1/2)  

(2) 2, 0,0,1/2  
     (2, 1/2,0,1/2)  

(3) 2, 1/2,0,1/2  
     (2, 1/2,0,1/2)  

(4) 2, 1/2,0,1/2  
     (2, 1/2,0,1/2)  

(5) $3$, (1/3,1/3,1/3)  
     x+1/3,x+1/3,x  
     (3, 0,1/2,1/2)  

(6) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(7) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(8) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(9) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(10) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(11) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(12) $\bar{3}$, x,x+1/2,x  
     (3, 0,1/2,1/2)  

(13) $\bar{1}$, 1/4,0,1/4  
     (1, 1/2,0,1/2)  

(14) $a$, 0,1/2,0  
     (a, 1/2,0,0,1/2)  

(15) $n$, 0,0,1/2  
     (n, 1/2,0,0,1/2)  

(16) $c$, 0,0,1/2  
     (c, 1/2,0,0,1/2)  

(17) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

(18) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

(19) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

(20) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

(21) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

(22) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

(23) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

(24) $\bar{3}$, x,x,x; 0,0,1/2  
     (3, 1/2,0,0,1/2)  

Continued

202.1.1524

Fm$\bar{3}$

202.1.1524 - 2 - 3382
For (1/2, 1/2, 0) + set

(1) \( t (1/2, 1/2, 0) \)
(2) \( 2 \ (1/2, 1/2, 0) \)
(3) \( 2 (0, 1/2, 0) \)
(4) \( 2 (1/2, 1/2, 0) \)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>96 i 1</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
</tbody>
</table>

Generators selected

(1); \( t(1,0,0) \); \( t(0,1,0) \); \( t(0,0,1) \); \( t(0,1/2,1/2) \); \( t(1/2,0,1/2) \); (2); (3); (5); (13).

Continued
Symmetry of Special Projections

Along [0,0,1] p2mm1'  
\[a^* = a/2\quad b^* = b/2\]  
Origin at 0,0,z

Along [1,1,1] p6'  
\[a^* = (2a - b - c)/6\quad b^* = (-a + 2b - c)/6\]  
Origin at x,x,x

Along [1,1,0] c2'mm'  
\[a^* = c\quad b^* = -(-a + b)/2\]  
Origin at x,x,0

48  
g 2..  
\[x,1/4,1/4 [u,0,0]\quad \bar{x},3/4,1/4 [\bar{u},0,0]\quad 1/4,x,1/4 [0,u,0]\]
\[1/4,\bar{x},3/4 [0,\bar{u},0]\quad 1/4,1/4,x [0,0,u]\quad 3/4,1/4,\bar{x} [0,0,\bar{u}]\]
\[\bar{x},3/4,3/4 [u,0,0]\quad x,1/4,3/4 [\bar{u},0,0]\quad 3/4,\bar{x},3/4 [0,u,0]\]
\[3/4,x,1/4 [0,\bar{u},0]\quad 3/4,3/4,\bar{x} [0,0,u]\quad 1/4,3/4,x [0,0,\bar{u}]\]

32  
f .3.  
\[x,x,x [u,u,u]\quad \bar{x},x,x [\bar{u},u,u]\quad \bar{x},x,x [u,\bar{u},u]\quad x,x,x [u,u,\bar{u}]\]

24  
e mm2..  
\[x,0,0 [0,0,0]\quad \bar{x},0,0 [0,0,0]\quad 0,x,0 [0,0,0]\]
\[0,\bar{x},0 [0,0,0]\quad 0,0,\bar{x} [0,0,0]\quad 0,0,\bar{x} [0,0,0]\]

24  
d 2/m..  
\[0,1/4,1/4 [u,0,0]\quad 0,3/4,1/4 [u,0,0]\quad 1/4,0,1/4 [0,u,0]\]
\[1/4,0,3/4 [0,\bar{u},0]\quad 1/4,1/4,0 [0,0,u]\quad 3/4,1/4,0 [0,0,\bar{u}]\]

8  
c 23.  
\[1/4,1/4,1/4 [0,0,0]\quad 3/4,3/4,3/4 [0,0,0]\]

4  
b m\bar{3}.  
\[1/2,1/2,1/2 [0,0,0]\]

4  
a m\bar{3}.  
\[0,0,0 [0,0,0]\]
Origin at center (m\overline{3}1')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z < \min (1/2-x,y) \]

Vertices

- 0,0,0
- 1/2,0,0
- 1/2,1/2,0
- 1/4,1/4,1/4

Symmetry Operations

For (0,0,0) + set

\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 2,0,0,0 \\
(2) & \quad 0,0,z \\
(3) & \quad 0,y,0 \\
(3) & \quad 2,0,0,0 \\
(4) & \quad 2,0,0 \\
(5) & \quad 3^+ x,x,x \\
(5) & \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ x,x,x \\
(6) & \quad (3_{xyz}|0,0,0) \\
(7) & \quad 3^+ x,x,x \\
(7) & \quad (3_{xyz}|0,0,0) \\
(8) & \quad 3^+ x,x,x \\
(8) & \quad (3_{xyz}|0,0,0) \\
(9) & \quad 3^+ x,x,x \\
(9) & \quad (3_{xyz}|0,0,0) \\
(10) & \quad 3^+ x,x,x \\
(10) & \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^+ x,x,x \\
(11) & \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^+ x,x,x \\
(12) & \quad (3_{xyz}|0,0,0) \\
\end{align*}

Continued

202.2.1525

202.2.1525 - 1 - 3385
(13) \( \frac{1}{3} 0,0,0 \)
(14) \( m \ x,y,0 \)
(15) \( m \ x,0,z \)
(16) \( m \ 0,y,z \)

(17) \( \frac{1}{3} x,x,x; 0,0,0 \)
(18) \( \frac{1}{3} x,x,x; 0,0,0 \)
(19) \( \frac{1}{3} x,x,x; 0,0,0 \)
(20) \( \frac{1}{3} x,x,x; 0,0,0 \)

(21) \( \frac{3}{5} x,x,x; 0,0,0 \)
(22) \( \frac{3}{5} x,x,x; 0,0,0 \)
(23) \( \frac{3}{5} x,x,x; 0,0,0 \)
(24) \( \frac{3}{5} x,x,x; 0,0,0 \)

For (0,1/2,1/2) + set

(1) \( t (0,1/2,1/2) \)
(2) \( t (0,1/2,1/2) \)
(3) \( t (0,1/2,1/2) \)
(4) \( t (0,1/2,1/2) \)

(5) \( 3 \frac{1}{2} (1/3,1/3,1/3) \)
(6) \( 3 \frac{1}{2} x,x+1/2,x \)
(7) \( 3 \frac{1}{2} x,x+1/2,x \)
(8) \( 3 \frac{1}{2} x,x+1/2,x \)

(9) \( 3 \frac{1}{2} (1/3,1/3,1/3) \)
(10) \( 3 \frac{1}{2} x,x+1/2,x \)
(11) \( 3 \frac{1}{2} x,x+1/2,x \)
(12) \( 3 \frac{1}{2} x,x+1/2,x \)

(13) \( \frac{1}{2} 0,1/4,1/4 \)
(14) \( \frac{1}{2} x,y,0 \)
(15) \( \frac{1}{2} x,0,z \)
(16) \( \frac{1}{2} 0,y,z \)

For (1/2,0,1/2) + set

(1) \( t (1/2,0,1/2) \)
(2) \( t (1/2,0,1/2) \)
(3) \( t (1/2,0,1/2) \)
(4) \( t (1/2,0,1/2) \)

(5) \( 3 \frac{1}{2} (1/3,1/3,1/3) \)
(6) \( 3 \frac{1}{2} x,x+1/2,x \)
(7) \( 3 \frac{1}{2} x,x+1/2,x \)
(8) \( 3 \frac{1}{2} x,x+1/2,x \)

(9) \( 3 \frac{1}{2} (1/3,1/3,1/3) \)
(10) \( 3 \frac{1}{2} x,x+1/2,x \)
(11) \( 3 \frac{1}{2} x,x+1/2,x \)
(12) \( 3 \frac{1}{2} x,x+1/2,x \)

(13) \( \frac{1}{2} 1/4,0,1/4 \)
(14) \( \frac{1}{2} x,y,0 \)
(15) \( \frac{1}{2} x,0,z \)
(16) \( \frac{1}{2} 0,y,z \)

Continued

202.2.1525
Fm \( \overline{3} 1' \)

202.2.1525 - 2 - 3386
(13) $\bar{T}$' 0,1/4,1/4 \\
(14) $b'(0,1/2,0)$ x,y,1/4 \\
(15) $c'(0,0,1/2)$ x,1/4,z \\
(16) $n'(0,1/2,1/2)$ 0,y,z \\
(17) $3^{*'} x,x+1/2$,x; \\
(18) $3^{*'} x,-1,x+1/2$,x; \\
(19) $3^{*'} x,x+1/2$,x; \\
(20) $3^{*'} x,-1,x+1/2$,x; \\
(21) $3^{*'} x,-1/2,x,-1/2$,x; \\
(22) $3^{*'} x+1/2,x,-1/2$,x; \\
(23) $3^{*'} x-1/2,x+1/2$,x; \\
(24) $3^{*'} x+1/2,x+1/2$,x; \\
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
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\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
\[
\left(\frac{3}{xyz}\right)|0,1/2,1/2)' \\
\]
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); 1'.

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
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<td>96  i 11'</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + (0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
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<tr>
<td>(5) z,x,y [0,0,0]</td>
<td>(6) z,x,y [0,0,0]</td>
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<tr>
<td>(9) y,z,x [0,0,0]</td>
<td>(10) y,z,x [0,0,0]</td>
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<td>(14) x,y,z [0,0,0]</td>
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<td>(18) x, y, z [0,0,0]</td>
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<td>(22) x, y, z [0,0,0]</td>
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<td>48  h m..1'</td>
<td>0,y,z [0,0,0]</td>
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<td>0,y,z [0,0,0]</td>
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<td>x,1/4,3/4 [0,0,0]</td>
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<td>32  f 3..1'</td>
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<tr>
<td></td>
<td>x,x,x [0,0,0]</td>
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<tr>
<td>24  e mm2..1'</td>
<td>x,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,x,0 [0,0,0]</td>
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<td>0,x,0 [0,0,0]</td>
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<td>24  d 2/m..1'</td>
<td>0,1/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>0,3/4,1/4 [0,0,0]</td>
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<tr>
<td>8   c 23.1'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
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<tr>
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<td>3/4,3/4,3/4 [0,0,0]</td>
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<tr>
<td>4   b m3.1'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4   a m3.1'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

Continued  202.2.1525 Fm31'
Symmetry of Special Projections

Along $[0,0,1]$ p2mm1'
$\mathbf{a}^* = \frac{a}{2}$  $\mathbf{b}^* = \frac{b}{2}$  $\mathbf{c}^* = \mathbf{c}$
Origin at 0,0,z

Along $[1,1,1]$ p61'
$\mathbf{a}^* = \frac{(2a - b - c)}{6}$  $\mathbf{b}^* = \frac{(-a + 2b - c)}{6}$  $\mathbf{c}^* = \frac{(-a + b)}{2}$
Origin at x,x,x

Along $[1,1,0]$ c2mm1'
$\mathbf{a}^* = \frac{(-a + b)}{2}$  $\mathbf{b}^* = \mathbf{c}$
Origin at x,x,0
Origin at center (m'3̅)

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ x; z ≤ min (1/2-x,y)

Vertices

0,0,0 1/2,0,0 1/2,1/2,0  1/4,1/4,1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 0,0,0)

(5) 3̅^+ x,x,x
(3_xyz|0,0,0)

(9) 3̅^+ x,x,x
(3_xyz^-1|0,0,0)

(2) 2 0,0,z
(2_z 0,0,0)

(6) 3^− x,x,x
(3_xyz^-1|0,0,0)

(10) 3^− x,x,x
(3_xyz|0,0,0)

(3) 2 0,y,0
(2_y 0,0,0)

(7) 3^− x,x,x
(3_xyz^-1|0,0,0)

(11) 3^− x,x,x
(3_xyz|0,0,0)

(4) 2 x,0,0
(2_x 0,0,0)

(8) 3^− x,x,x
(3_xyz^-1|0,0,0)

(12) 3^− x,x,x
(3_xyz|0,0,0)
For $(1/2,1/2,0) + set$

(1) $t$ (1/2,1/2,0)  
(1) $| 1/2,1/2,0)$

(2) $x$ (1/2,1/2,0)  
(2) $| 1/2,1/2,0)$

(1) $y$ (1/2,1/2,0)  
(1) $| 1/2,1/2,0)$

(3) $z$ (1/2,1/2,0)  
(3) $| 1/2,1/2,0)$

(4) $x$ (1/2,1/2,0)  
(4) $| 1/2,1/2,0)$

(5) $y$ (1/2,1/2,0)  
(5) $| 1/2,1/2,0)$

(6) $z$ (1/2,1/2,0)  
(6) $| 1/2,1/2,0)$

(7) $x$ (1/2,1/2,0)  
(7) $| 1/2,1/2,0)$

(8) $y$ (1/2,1/2,0)  
(8) $| 1/2,1/2,0)$

(9) $z$ (1/2,1/2,0)  
(9) $| 1/2,1/2,0)$

Continued 202.3.1526 Fm$3\bar{3}$

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<th>Wyckoff letter</th>
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<tr>
<td>96</td>
<td>$i$</td>
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<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
</tbody>
</table>

| Generators selected | (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13). |

| Generators selected | (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13). |

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
</tbody>
</table>

202.3.1526 - 3 - 3393
### Symmetry of Special Projections

| 48 g 2. | $x,1/4,1/4 [u,0,0]$ | $\bar{x},3/4,1/4 [\bar{u},0,0]$ | $1/4,x,1/4 [0,u,0]$ |
|-----------------------------------------------|
| | $1/4 , \bar{x},3/4 [0,\bar{u},0]$ | $1/4,1/4,x [0,0,u]$ | $3/4,1/4,\bar{x} [0,0,\bar{u}]$ |
| | $\bar{x},3/4,3/4 [\bar{u},0,0]$ | $x,1/4,3/4 [u,0,0]$ | $3/4 , \bar{x},3/4 [0,u,0]$ |
| | $3/4,x,1/4 [0,u,0]$ | $3/4,3/4,\bar{x} [0,0,\bar{u}]$ | $1/4,3/4,x [0,0,u]$ |

| 32 f .3. | $x,x,x [u,u,u]$ | $\bar{x},x,x [\bar{u},u,u]$ | $\bar{x},x,x [u,u,\bar{u}]$ |
|-----------------------------------------------|
| | $\bar{x},x,x [u,u,u]$ | $\bar{x},x,x [u,u,u]$ | $\bar{x},x,x [u,u,\bar{u}]$ |

| 24 e m'm'2. | $x,0,0 [u,0,0]$ | x,0,0 [u,0,0] | 0,x,0 [0,u,0] |
|-----------------------------------------------|
| | 0,x,0 [0,u,0] | 0,0,x [0,0,u] | 0,0,x [0,0,u] |

| 24 d 2/m'. | $0,1/4,1/4 [0,0,0]$ | 0,3/4,1/4 [0,0,0] | 1/4,0,1/4 [0,0,0] |
|-----------------------------------------------|
| | 1/4,0,3/4 [0,0,0] | 1/4,1/4,0 [0,0,0] | 3/4,1/4,0 [0,0,0] |

| 8 c 23. | $1/4,1/4,1/4 [0,0,0]$ | $3/4,3/4,3/4 [0,0,0]$ |
|-----------------------------------------------|

| 4 b m'3'. | $1/2,1/2,1/2 [0,0,0]$ |

| 4 a m'3'. | $0,0,0 [0,0,0]$ |

**Symmetry of Special Projections**

**Along [0,0,1] p2m'm'**

- $a^* = a/2$
- $b^* = b/2$

**Origin at 0,0,z**

**Along [1,1,1] p6**

- $a^* = (2a - b - c)/6$
- $b^* = (-a + 2b - c)/6$

**Origin at x,x,x**

**Along [1,1,0] c2m'm'**

- $a^* = (-a + b)/2$
- $b^* = c$

**Origin at x,x,0**

---

202.3.1526 - 4 - 3394
Fd\textsuperscript{3}  

203.1.1527  

Cubic

m\textsuperscript{3}  

F2/d\textsuperscript{3}  

Origin at 23, at -1/8,-1/8,-1/8 from center (3)

Asymmetric unit  

0 \leq x \leq 1/2;  
0 \leq y \leq 1/4;  
-1/4 \leq z \leq 1/4;  
y \leq \min(x,1/2-x);  
-y \leq z \leq y

Vertices  

0,0,0  
1/2,0,0  
1/4,1/4,1/4  
1/4,1/4,-1/4

Symmetry Operations

For (0,0,0) + set

(1) 1  

(1 | 0,0,0)  

(2) \text{2} 0,0,z  

(2_z | 0,0,0)  

(3) \text{2} y,0,0  

(2_y | 0,0,0)  

(4) \text{2} x,0,0  

(2_x | 0,0,0)  

(5) 3\text{'} x,x,x  

(3_{xyz} | 0,0,0)  

(6) 3\text{'} x,x,x  

(3_{xyz}^{-1} | 0,0,0)  

(7) 3\text{'} x,x,x  

(3_{xyz}^{-1} | 0,0,0)  

(8) 3\text{'} x,x,x  

(3_{xyz}^{-1} | 0,0,0)  

(9) 3\text{'} x,x,x  

(3_{xyz}^{-1} | 0,0,0)  

(10) 3\text{'} x,x,x  

(3_{xyz}^{-1} | 0,0,0)  

(11) 3\text{'} x,x,x  

(3_{xyz}^{-1} | 0,0,0)  

(12) 3\text{'} x,x,x  

(3_{xyz}^{-1} | 0,0,0)  

203.1.1527 - 1 - 3395
Continued

| (21) $\bar{3}$: x+1/2,x,x; | (22) $\bar{3}$: x+1,x-3/2,x; | (23) $\bar{3}$: x+1/2,x+3/2,x; | (24) $\bar{3}$: x+1,x,x; |
| 5/8,1/8,1/8 | 1/8,-5/8,7/8 | -1/8,7/8,5/8 | 7/8,1/8,-1/8 |
| $(\bar{3}_{xyz})^1|3/4,1/4,3/4|$ | $(\bar{3}_{xyz})|3/4,1/4,3/4|$ | $(\bar{3}_{xyz})|3/4,1/4,3/4|$ | $(\bar{3}_{xyz})|3/4,1/4,3/4|$ |

For $(1/2,1/2,0)+$ set

| (1) t $(1/2,1/2,0)$ | (2) 2 $1/4,1/4,z$ | (3) 2 $(0,1/2,0)$ | (4) 2 $(1/2,0,0)$ |
| (1) $1/2,1/2,0)$ | $(2_z)|1/2,1/2,0)$ | $(2_z)|1/2,1/2,0)$ | $(2_z)|1/2,1/2,0)$ |

| (5) $3^+ (1/3,1/3,1/3)$ | (6) $3^+ x+1/2,x,x$ | (7) $3^+ x+1/2,x,x$ | (8) $3^+ (1/3,1/3,-1/3)$ |
| $x+1/6,x+1/3,x$ | $(3_{xyz})|1/2,1/2,0)$ | $(3_{xyz})|1/2,1/2,0)$ | $(3_{xyz})|1/2,1/2,0)$ |

| (9) $3^+ (1/3,1/3,1/3)$ | (10) $3^+ x,x+1/2,x$ | (11) $3^+ (1/3,1/3,-1/3)$ | (12) $3^+ x+3/2,x$ |
| $x+1/3,x+1/6,x$ | $(3_{xyz})|1/2,1/2,0)$ | $(3_{xyz})|1/2,1/2,0)$ | $(3_{xyz})|1/2,1/2,0)$ |

| (13) $\bar{1} 3/8,3/8,1/8$ | (14) d $(3/4,3/4,0)$ x,y,1/8 | (15) d $(3/4,0,1/4)$ x,3/8,z | (16) d $(0,3/4,1/4)$ 3/8,y,z |
| $(\bar{1})|3/4,3/4,1/4|$ | $(m_z)|3/4,3/4,1/4|$ | $(m_y)|3/4,3/4,1/4|$ | $(m_z)|3/4,3/4,1/4|$ |

Continued

| (17) $\bar{3}^+ x+1/2,x,x;$ | (18) $\bar{3}^+ x-1,x+3/2,x;$ | (19) $\bar{3}^+ x-1/2,x+3/2,x;$ | (20) $\bar{3}^+ x+1,x,x;$ |
| 5/8,1/8,1/8 | -1/8,5/8,7/8 | 1/8,7/8,-5/8 | 7/8,-1/8,1/8 |
| $(\bar{3}_{xyz})|3/4,3/4,1/4|$ | $(\bar{3}_{xyz})|3/4,3/4,1/4|$ | $(\bar{3}_{xyz})|3/4,3/4,1/4|$ | $(\bar{3}_{xyz})|3/4,3/4,1/4|$ |

| (21) $\bar{3}^+ x,x+1/2,x;$ | (22) $\bar{3}^+ x+3/2,x-1,x;$ | (23) $\bar{3}^+ x,x+1,x;$ | (24) $\bar{3}^+ x+3/2,x-1/2,x;$ |
| 1/8,5/8,1/8 | 5/8,-1/8,7/8 | -1/8,7/8,1/8 | 7/8,1/8,-5/8 |
| $(\bar{3}_{xyz})|3/4,3/4,1/4|$ | $(\bar{3}_{xyz})|3/4,3/4,1/4|$ | $(\bar{3}_{xyz})|3/4,3/4,1/4|$ | $(\bar{3}_{xyz})|3/4,3/4,1/4|$ |

Generators selected

| (1); t$(1,0,0);$ t$(0,1,0);$ t$(0,0,1);$ t$(0,1/2,1/2);$ t$(1/2,0,1/2);$ (2); (3); (5); (13). |

Positions

<p>| Multiplicity, Wyckoff letter, Site Symmetry. |
| Coordinates |
| (0,0,0) + | (0,1/2,1/2) + | (1/2,0,1/2) + | (1/2,1/2,0) + |
| (1) x,y,z [u,v,w] | (2) $\bar{x},\bar{y},\bar{z}$ [u,v,w] | (3) $\bar{x},\bar{y},\bar{z}$ [u,v,w] | (4) x,y,z [u,v,w] |
| (5) z,x,y [w,u,v] | (6) z,x,y [w,u,v] | (7) z,x,y [w,u,v] | (8) z,x,y [w,u,v] |
| (9) y,z,x [v,w,u] | (10) y,z,x [v,w,u] | (11) y,z,x [v,w,u] | (12) y,z,x [v,w,u] |
| (13) $\bar{x}+1/4,y+1/4,\bar{z}+1/4$ [u,v,w] | (14) x+1/4,y+1/4,\bar{z}+1/4 [u,v,w] | (15) x+1/4,y+1/4,\bar{z}+1/4 [u,v,w] | (16) x+1/4,y+1/4,\bar{z}+1/4 [u,v,w] |
| (17) $\bar{z}+1/4,x+1/4,\bar{y}+1/4$ [w,u,v] | (18) $\bar{z}+1/4,x+1/4,\bar{y}+1/4$ [w,u,v] | (19) z+1/4,x+1/4,\bar{y}+1/4 [w,u,v] | (20) z+1/4,x+1/4,\bar{y}+1/4 [w,u,v] |
| (21) $\bar{y}+1/4,\bar{z}+1/4,x+1/4$ [v,w,u] | (22) $\bar{y}+1/4,\bar{z}+1/4,x+1/4$ [v,w,u] | (23) y+1/4,z+1/4,x+1/4 [v,w,u] | (24) y+1/4,z+1/4,x+1/4 [v,w,u] |</p>
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<th>48</th>
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<th>(\bar{x},0,0) [u,0,0]</th>
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<td>(0,\bar{x},0) [0,u,0]</td>
<td>(0,\bar{x},0) [0,u,0]</td>
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<td>(\bar{x}+1/4,1/4,1/4) [u,0,0]</td>
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<td>(\bar{x},\bar{x},\bar{x}) [u,u,u]</td>
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<td>(\bar{x}+1/4,x+1/4,\bar{x}+1/4) [u,u,u]</td>
<td>(\bar{x}+1/4,x+1/4,\bar{x}+1/4) [u,u,u]</td>
<td>(\bar{x}+1/4,x+1/4,\bar{x}+1/4) [u,u,u]</td>
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<td>(x+1/4,\bar{x}+1/4,\bar{x}+1/4) [u,u,u]</td>
<td>(x+1/4,\bar{x}+1/4,\bar{x}+1/4) [u,u,u]</td>
<td>(x+1/4,\bar{x}+1/4,\bar{x}+1/4) [u,u,u]</td>
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<td></td>
<td>(1/8,1/8,1/8) [u,u,u]</td>
<td>(7/8,1/8,1/8) [u,u,u]</td>
<td>(7/8,1/8,7/8) [u,u,u]</td>
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<tr>
<td>8</td>
<td>b 23.</td>
<td>(0,0,0) [0,0,0]</td>
<td>(1/4,1/4,1/4) [0,0,0]</td>
<td>(1/4,1/4,1/4) [0,0,0]</td>
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<tr>
<td>8</td>
<td>a 23.</td>
<td>(0,0,0) [0,0,0]</td>
<td>(1/4,1/4,1/4) [0,0,0]</td>
<td>(1/4,1/4,1/4) [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] \(c_p,2m'm'\)
\[a^* = a/2\quad b^* = b/2\]
Origin at 0,0,z

Along [1,1,1] \(p6'\)
\[a^* = (2a - b - c)/6\quad b^* = (-a + 2b - c)/6\]
Origin at x,x,x

Along [1,1,0] \(c2'mm'\)
\[a^* = c\quad b^* = (-a + b)/2\]
Origin at x,x,1/8
Fd\textsuperscript{3}1' \hspace{1cm} m\overline{3}\textsuperscript{1}' \hspace{1cm} \text{Cubic}

203.2.1528 \hspace{1cm} F2/d\overline{3}\textsuperscript{1}'

**Origin** at 231', at -1/8,-1/8,-1/8 from center (31')

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad -y \leq z \leq y \]

**Vertices**

\[ 0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4 \]

**Symmetry Operations**

For (0,0,0) + set

1. 1
   (1 | 0,0,0)

2. 2 0,0,z
   (2z | 0,0,0)

3. 2 0,y,0
   (2y | 0,0,0)

4. 2 x,0,0
   (2x | 0,0,0)

5. 3\textsuperscript{+} x,x,x
   (3_{xyz} | 0,0,0)

6. 3\textsuperscript{+} x,x,x
   (3_{xyz}^{-1} | 0,0,0)

7. 3\textsuperscript{+} x,x,x
   (3_{xyz}^{-1} | 0,0,0)

8. 3\textsuperscript{+} x,x,x
   (3_{xyz}^{-1} | 0,0,0)

9. 3\textsuperscript{-} x,x,x
   (3_{xyz}^{-1} | 0,0,0)

10. 3\textsuperscript{-} x,x,x
    (3_{xyz} | 0,0,0)

11. 3\textsuperscript{-} x,x,x
    (3_{xyz} | 0,0,0)

12. 3\textsuperscript{-} x,x,x
    (3_{xyz} | 0,0,0)
### Continued

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<tr>
<td>13</td>
<td>$\overline{1}$ 1/8,1/8,1/8</td>
<td>(14) d (1/4,1/4,0) x,y,1/8</td>
<td>(15) d (1/4,0,1/4) x,1/8,z</td>
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<tr>
<td>15</td>
<td>$\overline{1}$ 1/4,1/4,1/4</td>
<td>(m_x $\overline{1}$/4,1/4,1/4)</td>
<td>(m_y $\overline{1}$/4,1/4,1/4)</td>
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<tr>
<td>17</td>
<td>3' x,x,x; 1/8,1/8,1/8</td>
<td>(18) 3' $-x/2,x+1/2,x$;</td>
<td>(19) 3' $x,x+1/2,x$;</td>
</tr>
<tr>
<td>18</td>
<td>(3_xyz $1/4,1/4,1/4$)</td>
<td>$1/8,1/8,3/8$</td>
<td>$1/8,3/8,1/8$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3_xyz $-1/4,1/4,1/4$)</td>
<td>(3_xyz $-1/4,1/4,1/4$)</td>
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<tr>
<td>21</td>
<td>3' x,x,x; 1/8,1/8,1/8</td>
<td>(22) 3' $x+1/2,x+1/2,x$;</td>
<td>(23) 3' $x,x+1/2,x$;</td>
</tr>
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<td>22</td>
<td>(3_xyz $1/4,1/4,1/4$)</td>
<td>$1/8,-1/8,3/8$</td>
<td>$-1/8,3/8,1/8$</td>
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<tr>
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<td>(3_xyz $1/4,1/4,1/4$)</td>
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For (0,1/2,1/2) + set

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<td>(1) t (0,1/2,1/2)</td>
<td>(2) 2 (0,0,1/2) 0,1/4,z</td>
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<td>2</td>
<td>(1/2,0,1/2)</td>
<td>(2) 2 (0,1/2,1/2) 1/4,0,z</td>
<td>(3) 2 (0,1/2,0) 0,y,1/4</td>
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<tr>
<td></td>
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<td>(2_z $1/2,0,1/2$)</td>
<td>(2_y $1/2,0,1/2$)</td>
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<tr>
<td>5</td>
<td>3' (1/3,1/3,1/3) x+1/3,x-1/6,x</td>
<td>(6) 3' $x,x+1/2,$ $x$</td>
<td>(7) 3' (-1/3,1/3,1/3) $x+1/3,x-1/6,x$</td>
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<tr>
<td>6</td>
<td>(3_xyz $0,1/2,1/2$)</td>
<td>(3_xyz $1/2,0,1/2$)</td>
<td>(3_xyz $1/2,1/2$)</td>
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<td>(14) d (1/4,3/4,0) x,y,3/8</td>
<td>(15) d (1/4,0,3/4) x,3/8,z</td>
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<tr>
<td>17</td>
<td>3' x,x+1/2,x; 1/8,5/8,1/8</td>
<td>(18) 3' $x-3/2,x+1/2,$ $x$</td>
<td>(19) 3' $x,x+1/2,$ $x$</td>
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<td>(3_xyz $1/4,3/4,3/4$)</td>
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<td>$1/8,7/8,-1/8$</td>
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<tr>
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<td>3' x-1/2,x-1/2,x; 1/8,1/8,5/8</td>
<td>(22) 3' $x+1/2,x-1/2,$ $x$</td>
<td>(23) 3' $-x+1/2,x+1/2,$ $x$</td>
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<td>(3_xyz $1/4,3/4,3/4$)</td>
<td>$1/8,-1/8,7/8$</td>
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For (1/2,0,1/2) + set

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<td>(2) 2 (0,1/2,0) 1/4,0,z</td>
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<tr>
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<td>(1/2,0,1/2)</td>
<td>(2) 2 (1/2,0,1/2) 1,4,0,z</td>
<td>(3) 2 (1/2,0,1/2) 1/4,y,1/4</td>
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<td>(2_z $1/2,0,1/2$)</td>
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<th>For $(1/2,1/2,0)' + \text{set}$</th>
<th>203.2.1528</th>
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<td>$(1/2,0,1/2)'$</td>
<td>$d' (0,0,1/4)$</td>
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<td>$(1/2,1/2,0)'$</td>
<td>$(2) 2'(0,0,1/4)$</td>
<td>$1/4,0,1/4$</td>
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<tr>
<td>$(2) 2' (1/2,0,1/2)'$</td>
<td>$(2_1,1/2,0,1/2)'$</td>
<td>$x,0,1/4$</td>
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<td>$2' (1/2,1/2,0)$</td>
<td>$(3) 2' (1/4,0,1/4)$</td>
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<td>$(15) d' (1/4,0,3/4)$</td>
<td>$(16) d' (0,3/4,1/4)$</td>
<td>$1/8,1/2,1/8$</td>
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<td>$1/8,1/2,1/8$</td>
<td>$(17) 3' (1/3,1/3,1)$</td>
<td>$x+1/6,x+1/6,x$</td>
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<td>$(17) 3' (1/3,1/3,1)$</td>
<td>$(18) 3' (1/3,1/3,1)$</td>
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<td>$(19) 3' (1/3,1/3,1)$</td>
<td>$(20) 3' (1/3,1/3,1)$</td>
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<td>$(20) 3' (1/3,1/3,1)$</td>
<td>$(21) 3' (1/3,1/3,1)$</td>
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</table>
Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(0,1/2,1/2) +</td>
</tr>
<tr>
<td>(0,0,0)' +</td>
<td>(0,1/2,1/2)' +</td>
</tr>
<tr>
<td>(1/2,0,1/2) +</td>
<td>(1/2,0,1/2)' +</td>
</tr>
<tr>
<td>(1/2,1/2,0) +</td>
<td>(1/2,1/2,0)' +</td>
</tr>
</tbody>
</table>

96 g 11'

(1) x,y,z [0,0,0]
(2) x,y,z [0,0,0]
(3) x,y,z [0,0,0]
(4) x,y,z [0,0,0]
(5) z,x,y [0,0,0]
(6) z,x,y [0,0,0]
(7) z,x,y [0,0,0]
(8) z,x,y [0,0,0]
(9) z,x,y [0,0,0]
(10) z,x,y [0,0,0]
(11) z,x,y [0,0,0]
(12) z,x,y [0,0,0]
(13) x+1/4,y+1/4,z+1/4 [0,0,0]
(14) x+1/4,y+1/4,z+1/4 [0,0,0]
(15) x+1/4,y+1/4,z+1/4 [0,0,0]
(16) x+1/4,y+1/4,z+1/4 [0,0,0]
(17) x+1/4,y+1/4,z+1/4 [0,0,0]
(18) x+1/4,y+1/4,z+1/4 [0,0,0]
(19) x+1/4,y+1/4,z+1/4 [0,0,0]
(20) x+1/4,y+1/4,z+1/4 [0,0,0]
(21) x+1/4,y+1/4,z+1/4 [0,0,0]
(22) x+1/4,y+1/4,z+1/4 [0,0,0]
(23) x+1/4,y+1/4,z+1/4 [0,0,0]
(24) x+1/4,y+1/4,z+1/4 [0,0,0]

48 f 2..1'

x,0,0 [0,0,0]
0,0,x [0,0,0]
x+1/4,1/4,1/4 [0,0,0]
1/4,x+1/4,1/4 [0,0,0]

32 e .3.1'

x,x,x [0,0,0]
x,x,x [0,0,0]
x+1/4,x+1/4,x+1/4 [0,0,0]
x+1/4,x+1/4,x+1/4 [0,0,0]

16 d .3.1'

5/8,5/8,5/8 [0,0,0]
3/8,3/8,5/8 [0,0,0]
3/8,5/8,3/8 [0,0,0]
5/8,3/8,3/8 [0,0,0]

16 c .3.1'

1/8,1/8,1/8 [0,0,0]
7/8,7/8,1/8 [0,0,0]
7/8,1/8,7/8 [0,0,0]
1/8,7/8,7/8 [0,0,0]

8 b 23.1'

1/2,1/2,1/2 [0,0,0]
3/4,3/4,3/4 [0,0,0]

8 a 23.1'

0,0,0 [0,0,0]
1/4,1/4,1/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm1'

\( a^* = a/2 \quad b^* = b/2 \)

Origin at 0,0,z

Along [1,1,1] p61'

\( a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6 \)

Origin at x,x,x

Along [1,1,0] c2mm1'

\( a^* = (-a + b)/2 \quad b^* = c \)

Origin at x,x,1/8
Origin at 23, at -1/8,-1/8,-1/8 from center (3')

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad -y \leq z \leq y \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4 \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{array}{cccc}
(1) & 1 & (2) & 2 \ 0,0,z \\
(1 | 0,0,0) & (2_z | 0,0,0) \\
(5) & 3^+ x,x,x & (6) & 3^+ \ x, \ x, \ x \\
(3_{xyz} | 0,0,0) & (3_{xyz}^{-1} | 0,0,0) \\
(9) & 3^+ x,x,x & (10) & 3^+ \ x, \ x, \ x \\
(3_{xyz}^{-1} | 0,0,0) & (3_{xyz} | 0,0,0) \\
\end{array}
\]

\[
\begin{array}{cccc}
(3) & 2 \ 0,y,0 \\
(2_y | 0,0,0) \\
(7) & 3^+ x,x,x & (8) & 3^+ \ x, \ x, \ x \\
(3_{xyz}^{-1} | 0,0,0) & (3_{xyz}^{-1} | 0,0,0) \\
(11) & 3^+ x,x,x & (12) & 3^+ \ x, \ x, \ x \\
(3_{xyz} | 0,0,0) & (3_{xyz} | 0,0,0) \\
\end{array}
\]
Continued

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0) (2) 2' 1/4,1/4,z (3) 2' (0,1/2,0) 1/4,y,0 (4) 2' (1/2,0,0) x,1/4,0
(1 | 1/2,1/2,0) (2z | 1/2,1/2,0) (2y | 1/2,1/2,0) (2x | 1/2,1/2,0)

(5) 3' (1/3,1/3,1/3) (6) 3' x+1/2,x,x (7) 3' x+1/2,x,x (8) 3' (1/3,1/3,1/3)
x+1/6,x+1/3,x (3xyz | 1/2,1/2,0) (3xyz | 1/2,1/2,0) (3xyz | 1/2,1/2,0)

(9) 3' (1/3,1/3,1/3) (10) 3' x,x+1/2,x (11) 3' (1/3,1/3,1/3) x+1/3,x+1/6,x
(x+1/3,x+1/6,x (3xyz | 1/2,1/2,0) (3xyz | 1/2,1/2,0) (3xyz | 1/2,1/2,0)

(13) 1' 3/8,3/8,1/8 (14) d' (3/4,3/4,1/4) y,1/8 (15) d' (3/4,3/4,1/4) x,3/8,z (16) d' (0,3/4,1/4) 3/8,y,z
(1 | 3/4,3/4,1/4)' (17) 3++ x+1/2,x,x; (18) 3++ x-1,x+3/2,x; (19) 3++ x-1/2,x+3/2,x;
(5/8,1/8,1/8) (3xyz | 3/4,3/4,1/4)' (3xyz | 3/4,3/4,1/4)' (3xyz | 3/4,3/4,1/4)'

(21) 3'' x,x+1/2,x; (22) 3'' x+3/2,x-1,x; (23) 3'' x,x+1/2,x; (24) 3'' x+3/2,x-1/2,x;
(1/8,5/8,1/8) (3xyz | 3/4,3/4,1/4)' (3xyz | 3/4,3/4,1/4)' (3xyz | 3/4,3/4,1/4)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>96</th>
<th>g</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) z,x,y [w,u,v]</td>
<td>(7) z,x,y [w,u,v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) y,z,x [v,w,u]</td>
<td>(11) y,z,x [v,w,u]</td>
</tr>
<tr>
<td>(13) x+1/4,y+1/4,z+1/4 [u,v,w]</td>
<td>(14) x+1/4,y+1/4,z+1/4 [u,v,w]</td>
<td>(15) x+1/4,y+1/4,z+1/4 [u,v,w]</td>
</tr>
<tr>
<td>(17) z+1/4,x+1/4,y+1/4 [w,u,v]</td>
<td>(18) z+1/4,x+1/4,y+1/4 [w,u,v]</td>
<td>(19) z+1/4,x+1/4,y+1/4 [w,u,v]</td>
</tr>
<tr>
<td>(21) y+1/4,z+1/4,x+1/4 [v,w,u]</td>
<td>(22) y+1/4,z+1/4,x+1/4 [v,w,u]</td>
<td>(23) y+1/4,z+1/4,x+1/4 [v,w,u]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>48</th>
<th>f</th>
<th>2..</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
<td>x,0,0 [0,u,0]</td>
<td>x,0,0 [0,u,0]</td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
<td>x+1/4,1/4,1/4 [u,0,0]</td>
<td>x+1/4,1/4,1/4 [u,0,0]</td>
<td>1/4,x+1/4,1/4 [0,u,0]</td>
</tr>
<tr>
<td>1/4,x+1/4,1/4 [0,u,0]</td>
<td>1/4,x+1/4,1/4 [0,u,0]</td>
<td>1/4,x+1/4,1/4 [0,u,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>32</td>
<td>e</td>
<td>.3.</td>
<td>x,x,x [u,u,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>x,x,x [u,u,u]</td>
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<tr>
<td></td>
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<td></td>
<td>x+1/4,x+1/4,x+1/4 [u,u,u]</td>
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<td></td>
<td></td>
<td></td>
<td>x+1/4,x+1/4,x+1/4 [u,u,u]</td>
</tr>
<tr>
<td>16</td>
<td>d</td>
<td>.3'.</td>
<td>5/8,5/8,5/8 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/8,3/8,5/8 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
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<td>3/8,5/8,3/8 [0,0,0]</td>
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<td></td>
<td></td>
<td></td>
<td>5/8,3/8,3/8 [0,0,0]</td>
</tr>
<tr>
<td>16</td>
<td>c</td>
<td>.3'.</td>
<td>1/8,1/8,1/8 [0,0,0]</td>
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<td></td>
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<td>7/8,1/8,7/8 [0,0,0]</td>
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<td></td>
<td></td>
<td></td>
<td>1/8,7/8,7/8 [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>b</td>
<td>23.</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,3/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>a</td>
<td>23.</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/4,1/4,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

| Along [0,0,1] | c2m'm' |
| a' = a/2 | b' = b/2 |
| Origin at 0,0,z |

| Along [1,1,1] | p6 |
| a' = (2a - b - c)/6 | b' = (-a + 2b - c)/6 |
| Origin at x,x,x |

| Along [1,1,0] | c2m'm' |
| a' = (-a + b)/2 | b' = c |
| Origin at x,x,1/8 |
Origin at center (m3)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 1/2,1/2,1/2 \\
\end{align*}
\]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1 \mid 0,0,0) & \quad (2) \quad 2 \mid 0,0,z \\
(2_z \mid 0,0,0) & \quad (3) \quad 2 \mid 0,y,0 \\
(2_y \mid 0,0,0) & \quad (4) \quad 2 \mid x,0,0 \\
(2_z \mid 0,0,0) & \quad (5) \quad 3^+ \mid x,x,x \\
(3_{xyz} \mid 0,0,0) & \quad (6) \quad 3^+ \mid x,x,x \\
(3_{xyz}^{-1} \mid 0,0,0) & \quad (7) \quad 3^+ \mid x,x,x \\
(3_{xyz}^{-1} \mid 0,0,0) & \quad (8) \quad 3^+ \mid x,x,x \\
(3_{xyz}^{-1} \mid 0,0,0) & \quad (9) \quad 3^- \mid x,x,x \\
(3_{xyz} \mid 0,0,0) & \quad (10) \quad 3^- \mid x,x,x \\
(3_{xyz} \mid 0,0,0) & \quad (11) \quad 3^- \mid x,x,x \\
(3_{xyz} \mid 0,0,0) & \quad (12) \quad 3^- \mid x,x,x \\
\end{align*}
\]

Continued
Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13). \)

**Positions**

Multiplicty, Wyckoff letter, Site Symmetry.

48 \( h \ 1 \)

\begin{align*}
(1) & \quad x, y, z \ [u, v, w] \\
(5) & \quad z, x, y \ [w, u, v] \\
(9) & \quad y, z, x \ [v, w, u] \\
(13) & \quad x, y, z \ [u, v, w] \\
(17) & \quad z, x, y \ [w, u, v] \\
(21) & \quad y, z, x \ [v, w, u] \\
(14) & \quad m, x, y, 0 \ (m_z, 0, 0, 0) \\
(15) & \quad m, x, 0, z \ (m_y, 0, 0, 0) \\
(16) & \quad m, 0, y, z \ (m_x, 0, 0, 0) \\
(17) & \quad 3^+ \ x, x, x; 0, 0, 0 \ (3 \ \text{xyz}, 0, 0, 0) \\
(18) & \quad 3^+ \ \overline{x}, x, x; 0, 0, 0 \ (3 \ \text{xyz}^{-1}, 0, 0, 0) \\
(19) & \quad 3^+ \ x, x, x; 0, 0, 0 \ (3 \ \text{xyz}^{-1}, 0, 0, 0) \\
(20) & \quad 3^+ \ x, x, x; 0, 0, 0 \ (3 \ \text{xyz}^{-1}, 0, 0, 0) \\
(21) & \quad 3^- \ x, x, x; 0, 0, 0 \ (3 \ \text{xyz}^{-1}, 0, 0, 0) \\
(22) & \quad 3^- \ \overline{x}, x, \overline{x}; 0, 0, 0 \ (3 \ \text{xyz}, 0, 0, 0) \\
(23) & \quad 3^- \ x, x, x; 0, 0, 0 \ (3 \ \text{xyz}, 0, 0, 0) \\
(24) & \quad 3^- \ x, x, x; 0, 0, 0 \ (3 \ \text{xyz}, 0, 0, 0) \\
\end{align*}

For \( (1/2,1/2,1/2) + \) set

\begin{align*}
(1) & \quad t(1/2,1/2,1/2) \\
(2) & \quad 2(0,0,1/2) \ 1/4, 1/4, z \\
(3) & \quad 2(0,1/2,0) \ 1/4, y, 1/4 \\
(4) & \quad 2(1/2,0,0) \ x, 1/4, 1/4 \\
(5) & \quad 3^+ \ (1/2,1/2,1/2) \ x, x, x \\
(6) & \quad 3^+ \ (-1/6,1/6,1/6) \ x+1/3, x+3/3, x \\
(7) & \quad 3^+ \ 1/6, 1/6, 1/6 \ x+2/3, x-1/3, x \\
(8) & \quad 3^+ \ 1/6, 1/6, 1/6 \ x+1/3, x+2/3, x \\
(9) & \quad 3^- \ (1/2,1/2,1/2) \ x, x, x \\
(10) & \quad 3^- \ 1/6, 1/6, 1/6 \ x+1/3, x+3/3, x \\
(11) & \quad 3^- \ 1/6, 1/6, 1/6 \ x+2/3, x-1/3, x \\
(12) & \quad 3^- \ 1/6, 1/6, 1/6 \ x+1/3, x+2/3, x \\
(13) & \quad 3^- \ (1/2,1/2,1/2) \ x, x, x \\
(14) & \quad 3^- \ 1/2, 1/2, 1/2 \ x, x, x \\
(15) & \quad 3^- \ 1/2, 1/2, 1/2 \ x, x, x \\
(16) & \quad 3^- \ 1/2, 1/2, 1/2 \ x, x, x \\
(17) & \quad 3^+ \ (1/2,1/2,1/2) \ x, x, x \\
(18) & \quad 3^+ \ 1/4, 1/4, 1/4 \ x-1, x+1, x \\
(19) & \quad 3^+ \ 1/4, 1/4, 1/4 \ x-1, x+1, x \\
(20) & \quad 3^+ \ 1/4, 1/4, 1/4 \ x-1, x+1, x \\
(21) & \quad 3^- \ (1/2,1/2,1/2) \ x, x, x \\
(22) & \quad 3^- \ 1/2, 1/2, 1/2 \ x, x, x \\
(23) & \quad 3^- \ 1/2, 1/2, 1/2 \ x, x, x \\
(24) & \quad 3^- \ 1/2, 1/2, 1/2 \ x, x, x \\
\end{align*}

**Coordinates**

\( (0,0,0) + \ \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \) +
Continued

24  g  m..  0,y,z [u,0,0]  0,y,z [u,0,0]  0,y,z [u,0,0]
     0,y,z [u,0,0]  z,0,y [0,u,0]  z,0,y [0,u,0]
     z,0,y [0,u,0]  z,0,y [0,u,0]  y,z,0 [0,u,0]
     z,0,y [0,u,0]  y,z,0 [0,u,0]  y,z,0 [0,u,0]

16  f  .3.  x,x,x [u,u,u]  x,x,x [u,u,u]  x,x,x [u,u,u]
     x,x,x [u,u,u]  x,x,x [u,u,u]  x,x,x [u,u,u]

12  e  mm2..  x,0,1/2 [0,0,0]  1/2,x,0 [0,0,0]  1/2,x,0 [0,0,0]
     1/2,x,0 [0,0,0]  0,1/2,x [0,0,0]  0,1/2,x [0,0,0]

12  d  mm2..  x,0,0 [0,0,0]  0,x,0 [0,0,0]  0,x,0 [0,0,0]
     0,x,0 [0,0,0]  0,0,x [0,0,0]  0,0,x [0,0,0]


6   b  mmm..  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]

2   a  m3.  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  c2mm1'  a* = a  b* = b  Origin at 0,0,z
Along [1,1,1]  p6'  a* = (2a - b - c)/3  b* = (-a + 2b - c)/3  Origin at x,x,x
Along [1,1,0]  p2'mm'  a* = c/2  b* = -(a + b)/2  Origin at x,x,0
Origin at center (m\text{3}1')

Asymmetric unit

\begin{align*}
0 \leq x \leq 1/2; & \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y \\
\text{Vertices} & \quad 0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2
\end{align*}

Symmetry Operations

For \((0,0,0) + \text{set}

\begin{align*}
(1) 1 & \quad (2) 2 \quad 0,0,z \quad (3) 2 \quad 0,y,0 \\
(1 \mid 0,0,0) & \quad (2_z \mid 0,0,0) \quad (2_y \mid 0,0,0) \\
(5) 3^+ x,x,x & \quad (6) 3^+ \bar{x},x,\bar{x} \\
(3_{xyz} \mid 0,0,0) & \quad (3_{xyz}^{-1} \mid 0,0,0) \\
(9) 3^+ x,x,x & \quad (10) 3^+ \bar{x},\bar{x},\bar{x} \\
(3_{xyz}^{-1} \mid 0,0,0) & \quad (3_{xyz} \mid 0,0,0) \\
\text{Continued} & \quad (11) 3^+ \bar{x},\bar{x},x \\
& \quad (3_{xyz} \mid 0,0,0) \\
& \quad (12) 3^+ \bar{x},\bar{x},x \\
& \quad (3_{xyz}^{-1} \mid 0,0,0)
\end{align*}

204.2.1531 - 1 - 3411
For $(1/2,1/2,1/2)' + \text{set}$

(1) $t' (1/2,1/2,1/2)$

(2) $2' (0,0,1/2)$ 1/4,1/4,z

(3) $2' (0,1/2,0)$ 1/4,y,1/4

(4) $2' (1/2,0,0)$ x,1/4,1/4

(5) $3' (1/2,1/2,1/2) \times x,x,x$

(6) $3' (1/6,1,1,1/6) x+1/3,x+1/3,x$

(7) $3' (-1,6,1,1,1/6) x+2/3,x-1/3,x$

(8) $3' (1/6,1,1,1/6) x+1/3,x+2/3,x$

(9) $3' (1/2,1/2,1/2) \times x,x,x$

(10) $3' (-1,6,1,1,1/6) x+1/3,x+1/3,x$

(11) $3' (1,6,1,1,1/6) x+2/3,x+1/3,x$

(12) $3' (1/6,1,1,1/6) x+1/3,x+2/3,x$

(13) $3' (1/2,1/2,1/2) \times x,x,x$

(14) $3' (1/2,1/2,1/2) \times x,x,x$

(15) $3' (1/2,1/2,1/2) \times x,x,x$

(16) $3' (1/2,1/2,1/2) \times x,x,x$

(17) $3' (1/2,1/2,1/2) \times x,x,x$

(18) $3' (1/2,1/2,1/2) \times x,x,x$

(19) $3' (1/2,1/2,1/2) \times x,x,x$

(20) $3' (1/2,1/2,1/2) \times x,x,x$

(21) $3' (1/2,1/2,1/2) \times x,x,x$

(22) $3' (1/2,1/2,1/2) \times x,x,x$

(23) $3' (1/2,1/2,1/2) \times x,x,x$

(24) $3' (1/2,1/2,1/2) \times x,x,x$

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

48  h  11'

(1) x,y,z [0,0,0]

(2) $\bar{x},\bar{y},z [0,0,0]$

(3) $\bar{x},y,\bar{z} [0,0,0]$

(4) x,$\bar{y},z [0,0,0]$

(5) z,x,y [0,0,0]

(6) $z,\bar{x},\bar{y} [0,0,0]$

(7) $\bar{z},z,\bar{y} [0,0,0]$

(8) $\bar{z},z,\bar{y} [0,0,0]$

(9) y,z,x [0,0,0]

(10) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(11) $y,\bar{z},\bar{x} [0,0,0]$

(12) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(13) $\bar{x},\bar{y},\bar{z} [0,0,0]$

(14) x,$\bar{y},\bar{z} [0,0,0]$

(15) $x,\bar{y},\bar{z} [0,0,0]$

(16) $x,\bar{y},\bar{z} [0,0,0]$

(17) $\bar{z},\bar{x},\bar{y} [0,0,0]$

(18) $z,\bar{x},\bar{y} [0,0,0]$

(19) $\bar{z},\bar{x},\bar{y} [0,0,0]$

(20) $z,\bar{x},\bar{y} [0,0,0]$

(21) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(22) y,$\bar{z},\bar{x} [0,0,0]$

(23) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(24) $\bar{y},\bar{z},\bar{x} [0,0,0]$

Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

(25) x,y,z [0,0,0]

(26) $\bar{x},\bar{y},z [0,0,0]$

(27) $\bar{x},y,\bar{z} [0,0,0]$

(28) x,$\bar{y},z [0,0,0]$

(29) z,x,y [0,0,0]

(30) $z,\bar{x},\bar{y} [0,0,0]$

(31) $\bar{z},z,\bar{y} [0,0,0]$

(32) $\bar{z},z,\bar{y} [0,0,0]$

(33) y,z,x [0,0,0]

(34) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(35) $y,\bar{z},\bar{x} [0,0,0]$

(36) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(37) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(38) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(39) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(40) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(41) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(42) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(43) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(44) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(45) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(46) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(47) $\bar{y},\bar{z},\bar{x} [0,0,0]$

(48) $\bar{y},\bar{z},\bar{x} [0,0,0]$

Continued

204.2.1531  Im3 1'

204.2.1531 - 3 - 3413
<table>
<thead>
<tr>
<th>16</th>
<th>f</th>
<th>.3.1'</th>
<th>x,x,x [0,0,0]</th>
<th>x,x,x [0,0,0]</th>
<th>x,x,x [0,0,0]</th>
<th>x,x,x [0,0,0]</th>
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<td>12</td>
<td>e</td>
<td>mm2..1'</td>
<td>x,0,1/2 [0,0,0]</td>
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<td>1/2,x,0 [0,0,0]</td>
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<tr>
<td></td>
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<td>1/2 ,x,0 [0,0,0]</td>
<td>0,1/2,x [0,0,0]</td>
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<tr>
<td>12</td>
<td>d</td>
<td>mm2..1'</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
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<tr>
<td></td>
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<td>0,x,0 [0,0,0]</td>
<td>0,0,x [0,0,0]</td>
<td>0,0,x [0,0,0]</td>
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<tr>
<td>8</td>
<td>c</td>
<td>.3.1'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
<td>1/4,3/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td>mmm..1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>m3 1'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] c2mm1'  
\[a^* = a \quad b^* = b\]  
Origin at 0,0,z

Along [1,1,1] p61'  
\[a^* = \frac{2a - b - c}{3} \quad b^* = \frac{-a + 2b - c}{3}\]  
Origin at x,x,x

Along [1,1,0] p2mm1'  
\[a^* = \frac{-a + b}{2} \quad b^* = \frac{c}{2}\]  
Origin at x,x,0
Origin at center (m'3')

Asymmetric unit

\[0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/2; \quad y < x; \quad z < y\]

Vertices

\[0,0,0; \quad 1/2,0,0; \quad 1/2,1/2,0; \quad 1/2,1/2,1/2\]

Symmetry Operations

For \((0,0,0) + \text{ set}\)

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2,0,0,z \\
(3) & \quad 2,0,y,0 \\
(4) & \quad 2,x,0,0 \\
(5) & \quad 3^+ x,x,x \\
(6) & \quad 3^+ x,x,x \\
(7) & \quad 3^+ x,x,x \\
(8) & \quad 3^+ x,x,x \\
(9) & \quad 3^+ x,x,x \\
(10) & \quad 3^+ x,x,x \\
(11) & \quad 3^+ x,x,x \\
(12) & \quad 3^+ x,x,x \\
\end{align*}

Continued
For \((1/2,1/2,1/2) + \set\):

\[
\begin{align*}
(1) & \quad t (1/2,1/2,1/2) \\
(2) & \quad 2 (0,0,1/2) 1/4,1/4,z
\end{align*}
\]

Generators selected
(1) \(t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2);
(2); (3); (5); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

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\begin{align*}
(1) & \quad x,y,z [u,v,w] \\
(2) & \quad \bar{x},y,\bar{z} [\bar{u},\bar{v},\bar{w}] \\
(3) & \quad \bar{x},y,\bar{z} [\bar{u},\bar{v},w] \\
(4) & \quad x,y,\bar{z} [\bar{u},v,w] \\
(5) & \quad z,x,y [w,u,v] \\
(6) & \quad z,x,y [w,u,v] \\
(7) & \quad \bar{z},x,y [w,u,v] \\
(8) & \quad \bar{z},x,\bar{y} [w,u,v] \\
(9) & \quad y,z,x [v,w,u] \\
(10) & \quad \bar{y},z,\bar{x} [\bar{v},w,u] \\
(11) & \quad \bar{y},\bar{z},\bar{x} [\bar{v},w,u] \\
(12) & \quad \bar{y},z,\bar{x} [\bar{v},\bar{w},u] \\
(13) & \quad \bar{z},x,\bar{y} [\bar{u},v,w] \\
(14) & \quad \bar{z},x,\bar{y} [\bar{u},v,w] \\
(15) & \quad \bar{z},x,\bar{y} [\bar{u},v,w] \\
(16) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(17) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(18) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(19) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(20) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(21) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(22) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(23) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
(24) & \quad \bar{z},x,\bar{y} [\bar{u},\bar{v},w] \\
\end{align*}

Coordinates

\((0,0,0) + (1/2,1/2,1/2) + \)
Continued

24 g m'.. 0,y,z [0,v,w] 0,y,z [0,v,w] 0,y,z [0,v,w]
0,y,z [0,v,w] z,0,y [w,0,v] z,0,y [w,0,v]
\bar{z},0,y [w,0,v] \bar{z},0,y [w,0,v] y,z,0 [v,w,0]
y,z,0 [v,w,0] y,z,0 [v,w,0] \bar{y},z,0 [\bar{v},w,0]
\bar{y},z,0 [\bar{v},w,0] \bar{y},z,0 [\bar{v},w,0] \bar{y},z,0 [\bar{v},w,0]

16 f .3. x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]
x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]

12 e m'm'2.. x,0,1/2 [u,0,0] 1/2,x,0 [u,0,0] 1/2,x,0 [u,0,0]
1/2,x,0 [u,0,0] 0,1/2,x [0,0,u] 0,1/2,x [0,0,u]

12 d m'm'2.. x,0,0 [u,0,0] 0,x,0 [0,0,u] 0,x,0 [0,0,u]
0,x,0 [0,0,u] 0,0,x [0,0,u] 0,0,x [0,0,u]

8 c \bar{3}'. 1/4,1/4,1/4 [0,0,0] 3/4,3/4,1/4 [0,0,0] 3/4,3/4,1/4 [0,0,0] 1/4,3/4,3/4 [0,0,0]

6 b m'm'm'.. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,0,1/2 [0,0,0]

2 a m'3'. 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2m'm'
\textbf{a}^* = a \textbf{b}^* = b
Origin at 0,0,z

Along [1,1,1] p6
\textbf{a}^* = (2a - b - c)/3 \textbf{b}^* = (-a + 2b - c)/3
Origin at x,x,x

Along [1,1,0] p2m'm'
\textbf{a}^* = (-a + b)/2 \textbf{b}^* = c/2
Origin at x,x,0

204.3.1532 - 3 - 3417
Origin at center (m3)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2 \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
\text{(1) } & 1 \\
\text{(1) } & (1 | 0,0,0) \\
\text{(2) } & 2 \ 0,0,z \\
\text{(2) } & (2z | 0,0,0) \\
\text{(3) } & 2 \ 0,y,0 \\
\text{(3) } & (2y | 0,0,0) \\
\text{(4) } & 2 \ x,0,0 \\
\text{(4) } & (2x | 0,0,0) \\
\text{(5) } & 3^+ \ x,x,x \\
\text{(5) } & (3_{xyz} | 0,0,0) \\
\text{(6) } & 3^+ \bar{x},x,\bar{x} \\
\text{(6) } & (3_{xyz}^{-1} | 0,0,0) \\
\text{(7) } & 3^+ \bar{x},\bar{x},x \\
\text{(7) } & (3_{xyz}^{-1} | 0,0,0) \\
\text{(8) } & 3^+ \bar{x},\bar{x},x \\
\text{(8) } & (3_{xyz}^{-1} | 0,0,0) \\
\text{(9) } & 3^+ \ x,x,x \\
\text{(9) } & (3_{xyz}^{-1} | 0,0,0) \\
\text{(10) } & 3^+ \bar{x},\bar{x},\bar{x} \\
\text{(10) } & (3_{xyz}^{-1} | 0,0,0) \\
\text{(11) } & 3^+ \bar{x},\bar{x},x \\
\text{(11) } & (3_{xyz}^{-1} | 0,0,0) \\
\text{(12) } & 3^+ \bar{x},\bar{x},x \\
\text{(12) } & (3_{xyz}^{-1} | 0,0,0) \\
\end{align*}
\]

Continued
(13) $\bar{1}$ 0,0,0  \\
(14) m x,y,0  \\
(15) m x,0,z  \\
(16) m 0,y,z

(17) $3^*$ x,x;x 0,0,0  \\
(18) $3^*$ x,x,x 0,0,0  \\
(19) $3^*$ x,x,x 0,0,0

(21) $3^*$ x,x;x 0,0,0  \\
(22) $3^*$ x,x,x 0,0,0  \\
(23) $3^*$ x,x,x 0,0,0

For $(1/2,1/2,1/2)' + \text{set}$

(1) $t'$ (1/2,1/2,1/2)  \\
(2) $t'$ (0,0,1/2)  \\
(3) $t'$ (0,1/2,0)  \\
(4) $t'$ (1/2,0,0)  \\
(5) $3^*$ (1/2,1/2,1/2) x,x,x  \\
(6) $3^*$ (1/6,-1/6,1/6) x+1/3,x+1/3,x  \\
(7) $3^*$ (-1/6,1/6,1/6) x+2/3,x-1/3,x  \\
(8) $3^*$ (1/6,1/6,-1/6) x+1/3,x+2/3,x  \\
(9) $3^*$ (1/2,1/2,1/2) x,x,x  \\
(10) $3^*$ (-1/6,1/6,1/6) x+1/3,x+1/3,x  \\
(11) $3^*$ (-1/6,1/6,-1/6) x+2/3,x+1/3,x  \\
(12) $3^*$ (1/6,-1/6,1/6) x-1/3,x+2/3,x  \\
(13) $\bar{1}$ 1/4,1/4,1/4  \\
(14) n' (1/2,1/2,0) x,y,1/4  \\
(15) n' (1/2,0,1/2) x,1/4,z  \\
(16) n' (0,1/2,1/2) 1/4,y,z  \\
(17) $3^*$ x,x,x;  \\
1/4,1/4,1/4  \\
(18) $3^*$ -x,-x+1,-x;  \\
1/4,1/4,3/4  \\
(19) $3^*$ x,x+1,x;  \\
1/4,3/4,-1/4  \\
(20) $3^*$ x+1,x,x;  \\
3/4,-1/4,1/4

(21) $3^*$ x,x,x;  \\
1/4,1/4,1/4  \\
(22) $3^*$ x+1,-x+1,-x;  \\
1/4,-1/4,3/4  \\
(23) $3^*$ x,x+1,x;  \\
1/4,3/4,1/4  \\
(24) $3^*$ x+1,x,-x;  \\
3/4,1/4,-1/4

Generators selected
(1); (1,0,0); (0,1,0); (0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity,  
Wyckoff letter,  
Site Symmetry.

$48 \ h \ 1$

(1) x,y,z [u,v,w]  \\
(2) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$  \\
(3) $x,y,z [u,v,w]$  \\
(4) $x,y,\bar{z} [u,\bar{v},\bar{w}]$

(5) z,x,y [w,u,v]  \\
(6) z,x,y [w,u,v]  \\
(7) $\bar{z},x,y [w,u,v]$  \\
(8) $z,x,\bar{y} [w,u,\bar{v}]$

(9) y,z,x [v,w,u]  \\
(10) $\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$  \\
(11) y,z,x [v,w,u]  \\
(12) $\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$

(13) $\bar{x},y,\bar{z} [u,v,w]$  \\
(14) $\bar{x},y,\bar{z} [u,v,w]$  \\
(15) x,y,z [u,v,w]  \\
(16) x,y,z [u,v,w]

(17) $\bar{z},x,y [w,u,v]$  \\
(18) $\bar{z},x,y [w,u,v]$  \\
(19) z,x,\bar{y} [w,u,v]  \\
(20) z,x,\bar{y} [w,u,v]

(21) $\bar{y},\bar{z},\bar{x} [v,w,u]$  \\
(22) $\bar{y},\bar{z},\bar{x} [v,w,u]$  \\
(23) y,z,x [v,w,u]  \\
(24) $\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$

Continued 204.4.1533  \\
Continued 204.4.1533 - 2 - 3419

$204.4.1533 \ I_{p} m\bar{3}$
24 g m.. 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0]
0,y,z [u,0,0] z,0,y [0,u,0] z,0,y [0,u,0]
3,0,y [u,0,0] 3,0,y [u,0,0] y,z,0 [0,0,u] y,z,0 [0,0,u]

16 f 3. x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]
 x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]

12 e mm2.. x,0,1/2 [0,0,0] 1/2,x,0 [0,0,0] 1/2,x,0 [0,0,0]
1/2,x,0 [0,0,0] 0,1/2,x [0,0,0] 0,1/2,x [0,0,0]
1/2,x,0 [0,0,0] 0,1/2,x [0,0,0] 0,1/2,x [0,0,0]

12 d mm2.. x,0,0 [0,0,0] 0,x,0 [0,0,0] 0,x,0 [0,0,0]
0,x,0 [0,0,0] 0,0,x [0,0,0] 0,0,x [0,0,0]
0,x,0 [0,0,0] 0,0,x [0,0,0] 0,0,x [0,0,0]

8 c 3'. 1/4,1/4,1/4 [0,0,0] 3/4,3/4,1/4 [0,0,0] 3/4,1/4,3/4 [0,0,0] 1/4,3/4,3/4 [0,0,0]
6 b mmm.. 0,1/2,1/2 [0,0,0] 1/2,0,1/2 [0,0,0] 1/2,1/2,0 [0,0,0]

2 a m3. 0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] c2mm1' Along [1,1,1] p61' Along [1,1,0] p2a' 2mm
a* = a, b* = b a* = (2a - b - c)/3 b* = (-a + 2b - c)/3 a* = c/2 b* = (-a + b)/2
Origin at 0,0,z Origin at x,x,x Origin at x-1/4,x+1/4,0

204.4.1533 - 3 - 3420
Origin at center ($m'3'$)

Asymmetric unit

$x: 0 \leq x \leq 1/2$

$y: 0 \leq y < 1/2$

$z: 0 \leq z < 1/2$

$y: y < x$

$z: z < y$

Vertices

$0,0,0$

$1/2,0,0$

$1/2,1/2,0$

$1/2,1/2,1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$

2. $2,0,0,z$

3. $2,0,y,0$

4. $2,x,0,0$

5. $3^+ x,x,x$

6. $3^+ x,x,x$

7. $3^+ x,x,x$

8. $3^+ x,x,x$

9. $3^+ x,x,x$

10. $3^+ x,x,x$

11. $3^+ x,x,x$

12. $3^+ x,x,x$

Continued on the next page.
Positions selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

Coordinates

Multiplicity, Wyckoff letter, Site Symmetry:

48 h 1

(0,0,0) + (1/2,1/2,1/2)' +

(1) x,y,z [u,v,w]  
(2) x-x, z-y, z [u,v,w]  
(3) x,y,z [u,v,w]  
(4) x,y,z [u,v,w]  

(5) z,x,y [w,u,v]  
(6) z-x, y-y, y [w,u,v]  
(7) z,x,y [w,u,v]  
(8) z,x,y [w,u,v]  

(9) y,z,x [v,w,u]  
(10) y-z,x [v,w,u]  
(11) y,z,x [v,w,u]  
(12) y,z,x [v,w,u]  

(13) x,y,z [u,v,w]  
(14) x,y,z [u,v,w]  
(15) x,y,z [u,v,w]  
(16) x,y,z [u,v,w]  

(17) z,x,y [w,u,v]  
(18) z,x,y [w,u,v]  
(19) z,x,y [w,u,v]  
(20) z,x,y [w,u,v]  

(21) y,z,x [v,w,u]  
(22) y,z,x [v,w,u]  
(23) y,z,x [v,w,u]  
(24) y,z,x [v,w,u]  

Continued

204.5.1534

l, m, 3′
Symmetry of Special Projections

Along [0,0,1] \(c_p\) 2m'm'
\[a^* = a, b^* = b\]
Origin at 0,0,z

Along [1,1,1] p61'
\[a^* = (2a - b - c)/3, b^* = (-a + 2b - c)/3\]
Origin at x,x,x

Along [1,1,0] \(p_{3a}\) 2m'm'
\[a^* = (-a + b)/2, b^* = c/2\]
Origin at x,x,0
Pa3

Cubic

205.1.1535

P21/a3

Origin at center (3)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min (x,y) \]

Vertices

0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2

Symmetry Operations

(1) 1

(1 | 0,0,0)

(2) 2 (0,0,1/2) \quad 1/4,0,z

(2z | 1/2,0,1/2)

(3) 2 (0,1/2,0) \quad 0,y,1/4

(2y | 0,1/2,1/2)

(4) 2 (1/2,0,0) \quad x,1/4,0

(2x | 1/2,1/2,0)

(5) 3+ x,x,x

(3xyz | 0,0,0)

(6) 3+ x+1/2,x,x

(3xyz^{-1} | 1/2,1/2,0)

(7) 3+ x+1/2,x-1/2,x

(3xyz^{-1} | 1/2,0,1/2)

(8) 3+ x,x+1/2,x

(3xyz^{-1} | 0,1/2,1/2)

(9) 3- x,x,x

(3xyz^{-1} | 0,0,0)

(10) 3- (-1/3,1/3,1/3)

x+1/6,x+1/6,x

(3xyz | 0,1/2,1/2)

(11) 3- (1/3,1/3,-1/3)

x+1/3,x+1/6,x

(3xyz | 1/2,1/2,0)

(12) 3- (1/3,-1/3,1/3)

x-1/6,x+1/3,x

(3xyz | 1/2,0,1/2)
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 d 1

(1) x,y,z \[u,v,w\] (2) x+1/2,y,z+1/2 \[u,v,w\] (3) x,y+1/2,z+1/2 \[u,v,w\] (4) x+1/2,y+1/2,z \[u,v,w\]

Along [0,0,1] \( p_{2g} \), 2mg
\( a^* = b \) \( b^* = -a/2 \)
Origin at 0,0,z

8 c .3. x,x,x \[u,u,u\] x,x,x \[u,u,u\] x+1/2,x+1/2 \[u,u,u\] x+1/2,x+1/2 \[u,u,u\] x+1/2,x+1/2 \[u,u,u\]

4 b .3. 1/2,1/2,1/2 \[u,u,u\] 0,1/2,0 \[u,u,u\] 1/2,0,0 \[u,u,u\] 0,1/2 \[u,u,u\] 0,1/2 \[u,u,u\]

4 a .3. 0,0,0 \[u,u,u\] 1/2,0,1/2 \[u,u,u\] 0,1/2,1/2 \[u,u,u\] 1/2,1/2,0 \[u,u,u\]

Symmetry of Special Projections

Along [0,0,1] \p_{2g}, 2mg\n\( a^* = b \) \( b^* = -a/2 \)
Origin at 0,0,z

Along [1,1,1] \p_{6}'\n\( a^* = (2a-b-c)/3 \) \( b^* = (-a+2b-c)/3 \)
Origin at x,x,x

Along [1,1,0] \p_{2g}'\n\( a^* = -a + b)/2 \) \( b^* = c \)
Origin at x,x,0

205.1.1535 - 2 - 3425
### Symmetry Operations

**Origin** at center (3 1’)

**Asymmetric unit**

- $0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$; $z \leq \min(x,y)$

**Vertices**

- $(0,0,0)$
- $(1/2,0,0)$
- $(1/2,1/2,0)$
- $(0,1/2,0)$
- $(1/2,1/2,1/2)$

**Symmetry Operations**

For 1 + set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Matrix</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>$1$</td>
<td></td>
</tr>
<tr>
<td>(1</td>
<td>$0,0,0$</td>
<td></td>
</tr>
<tr>
<td>(2) 2</td>
<td>$0,0,1/2$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>$(2</td>
<td>z/2</td>
<td>$1/2,0,1/2$</td>
</tr>
<tr>
<td>(3) 2</td>
<td>$(0,1/2,0)$</td>
<td>$0,y,1/4$</td>
</tr>
<tr>
<td>$(2</td>
<td>y/2</td>
<td>$0,1/2,1/2$</td>
</tr>
<tr>
<td>(4) 2</td>
<td>$(1/2,0,0)$</td>
<td>$x,1/4,0$</td>
</tr>
<tr>
<td>$(2</td>
<td>x/2</td>
<td>$1/2,1/2,0$</td>
</tr>
<tr>
<td>(5) $3^+$</td>
<td>$x,y,z$</td>
<td>$x+1/2$</td>
</tr>
<tr>
<td>$(3</td>
<td>x/2</td>
<td>$x+1/2,0,1/2$</td>
</tr>
<tr>
<td>(6) $3^+$</td>
<td>$x+1/2,x$</td>
<td>$x+1/2,1/2,0$</td>
</tr>
<tr>
<td>$(3</td>
<td>x/2</td>
<td>$x+1/2,1/2,0$</td>
</tr>
<tr>
<td>(7) $3^+$</td>
<td>$x,y,z$</td>
<td>$x+1/2$</td>
</tr>
<tr>
<td>$(3</td>
<td>x/2</td>
<td>$x+1/2,0,1/2$</td>
</tr>
<tr>
<td>(8) $3^+$</td>
<td>$x,y,z$</td>
<td>$x+1/2$</td>
</tr>
<tr>
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<td>x/2</td>
<td>$x+1/2,1/2,0$</td>
</tr>
<tr>
<td>(9) $3^-$</td>
<td>$x,y,z$</td>
<td>$x-1/2$</td>
</tr>
<tr>
<td>$(3</td>
<td>x/2</td>
<td>$x-1/2,0,1/2$</td>
</tr>
<tr>
<td>(10) $3^-$</td>
<td>$x+1/6,x+1/6$</td>
<td>$x+1/6,0,1/2$</td>
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<tr>
<td>$(3</td>
<td>x/2</td>
<td>$x+1/6,0,1/2$</td>
</tr>
<tr>
<td>(11) $3^-$</td>
<td>$x+1/3,x+1/6$</td>
<td>$x+1/3,0,1/2$</td>
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<tr>
<td>$(3</td>
<td>x/2</td>
<td>$x+1/3,0,1/2$</td>
</tr>
<tr>
<td>(12) $3^-$</td>
<td>$(1/3,-1/3,1/3)$</td>
<td>$x-1/6,x+1/3$</td>
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<tr>
<td>$(3</td>
<td>x/2</td>
<td>$x-1/6,0,1/2$</td>
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</tbody>
</table>

Continued

205.2.1536
(13) \( \bar{1} \) 0,0,0  
(1\bar{1}) 0,0,0  
(1) 0,0,0  
(1') 0,0,0

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity,</td>
<td></td>
</tr>
<tr>
<td>Wyckoff letter,</td>
<td></td>
</tr>
<tr>
<td>Site Symmetry.</td>
<td></td>
</tr>
<tr>
<td>24  d 11'</td>
<td></td>
</tr>
</tbody>
</table>

(1) x,y,z [0,0,0]  
(2) \( x+1/2, y, z+1/2 \) [0,0,0]  
(3) \( x, y+1/2, z+1/2 \) [0,0,0]  
(4) \( x+1/2, y+1/2, z \) [0,0,0]  
(5) z,x,y [0,0,0]  
(6) \( z+1/2, x+1/2, y \) [0,0,0]  
(7) \( z+1/2, x, y+1/2 \) [0,0,0]  
(8) \( z, x+1/2, y+1/2 \) [0,0,0]  
(9) y,z,x [0,0,0]  
(10) \( y, z+1/2, x+1/2 \) [0,0,0]  
(11) \( y+1/2, z+1/2, x \) [0,0,0]  
(12) \( y+1/2, z, x+1/2 \) [0,0,0]  
(13) \( x, y, z \) [0,0,0]  
(14) \( x+1/2, y, z+1/2 \) [0,0,0]  
(15) \( x, y+1/2, z+1/2 \) [0,0,0]  
(16) \( x+1/2, y+1/2, z \) [0,0,0]  
(17) \( z, x, y \) [0,0,0]  
(18) \( z+1/2, x+1/2, y \) [0,0,0]  
(19) \( z+1/2, x, y+1/2 \) [0,0,0]  
(20) \( z, x+1/2, y+1/2 \) [0,0,0]  
(21) \( y, z, x \) [0,0,0]  
(22) \( y, z+1/2, x+1/2 \) [0,0,0]  
(23) \( y+1/2, z+1/2, x \) [0,0,0]  
(24) \( y+1/2, z, x+1/2 \) [0,0,0]  

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at x,x,x</th>
<th>Origin at x,x,x</th>
<th>Origin at x,x,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x,x [0,0,0]</td>
<td>x+1/2,x,x+1/2</td>
<td>x+1/2,x+1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>x+1/2,x,x+1/2</td>
<td>x,x+1/2,x+1/2</td>
<td>x+1/2,x+1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>x+1/2,x,x+1/2</td>
<td>x,x+1/2,x+1/2</td>
<td>x+1/2,x+1/2,x+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

#### Along [0,0,1] p2mg1'

- \( a^* = b \quad b^* = -a/2 \)
- Origin at 0,0,z

#### Along [1,1,1] p61'

- \( a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \)
- Origin at x,x,x

#### Along [1,1,0] p2gg1'

- \( a^* = (-a + b)/2 \quad b^* = c \)
- Origin at x,x,0
Origin at center (3\*)

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; z ≤ min (x,y)

Vertices  
0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/2,1/2,1/2

Symmetry Operations

(1) 1  
(1|0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z  
(2z|1/2,0,1/2)

(3) 2 (0,1/2,0) 0,y,1/4  
(2y|0,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0  
(2z|1/2,1/2,0)

(5) 3\* x,x,x  
(3xy|0,0,0)

(6) 3\* x+1/2,x,\overline{x}  
(3xy|1/2,1/2,0)

(7) 3\* x+1/2,\overline{x}-1/2,\overline{x}  
(3xy|1/2,0,1/2)

(8) 3\* \overline{x},x+1/2,\overline{x}  
(3xy|0,1/2,1/2)

(9) 3\* x,x,x  
(3xy|0,0,0)

(10) 3\* -1/3,1/3,1/3  
(3xy|0,1/2,1/2)

(11) 3\* 1/3,1/3,-1/3  
(3xy|1/2,1/2,0)

(12) 3\* 1/3,-1/3,1/3  
(3xy|1/2,0,1/2)

205.3.1537 - 1 - 3429
Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>24</th>
<th>d</th>
<th>1</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(2)</td>
<td>x+1/2,y+1/2,z+1/2</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(3)</td>
<td>x,y+1/2,z+1/2</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(4)</td>
<td>x+1/2,y+1/2,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>5</td>
<td>z,x,y</td>
<td>[w,u,v]</td>
</tr>
<tr>
<td>(6)</td>
<td>z+1/2,x+1/2,y</td>
<td>[w,u,v]</td>
</tr>
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<td>(7)</td>
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<td>[w,u,v]</td>
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<td>(8)</td>
<td>z,x+1/2,y+1/2</td>
<td>[w,u,v]</td>
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<tr>
<td>(9)</td>
<td>y,z,x</td>
<td>[v,w,u]</td>
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<tr>
<td>(10)</td>
<td>y,z+1/2,x+1/2</td>
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<td>y+1/2,z+1/2,x</td>
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<td>y+1/2,z,x+1/2</td>
<td>[v,w,u]</td>
</tr>
<tr>
<td>13</td>
<td>x,y,z</td>
<td>[u,v,w]</td>
</tr>
<tr>
<td>(14)</td>
<td>x+1/2,y,z+1/2</td>
<td>[u,v,w]</td>
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<td>[u,v,w]</td>
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<td>[v,w,u]</td>
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<tr>
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<td>[v,w,u]</td>
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<td>[v,w,u]</td>
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<td>21</td>
<td>y,z,x</td>
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<tr>
<td>(24)</td>
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<td>[v,w,u]</td>
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</table>

8 | c | .3. |
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<tr>
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<tbody>
<tr>
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4 | b | .3'. |
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4 | a | .3'. |
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<tr>
<td>0,0,0</td>
<td>[0,0,0]</td>
<td></td>
</tr>
<tr>
<td>1/2,0,1/2</td>
<td>[0,0,0]</td>
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<tr>
<td>1/2,1/2,0</td>
<td>[0,0,0]</td>
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<tr>
<td>1/2,1/2,0</td>
<td>[0,0,0]</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1]: p2m'g'

a* = b  b* = -a/2
Origin at 0,0,z

Along [1,1,1]: p6
a* = (2a - b - c)/3  b* = (-a + 2b - c)/3
Origin at x,x,x

Along [1,1,0]: p2g'g'
a* = (-a + b)/2  b* = c
Origin at x,x,0
**Origin at center (\&)**

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min (x,y)\]

**Vertices**

\[0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2\]

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

\begin{align*}
1 & \quad (1^0,0,0) \\
2 & \quad (2,0,0,1/2) \quad 1/4,0,z \\
3 & \quad (2,0,1/2,0,1/2) \quad 0,y,1/4 \\
4 & \quad (2,0,1/2,1/2,0) \quad x,1/4,0 \\
5 & \quad (3,0,0,0) \quad 1/2,0,1/2 \\
6 & \quad (3,0,1/2,0) \quad 0,1/2,1/2 \\
7 & \quad (3,0,1/2,1/2,0) \quad x,1/4,0 \\
8 & \quad (3,0,1/2,2,1/2,0) \quad x,1/4,0 \\
9 & \quad (3,0,1/2,2,1/2,0) \quad x,1/4,0 \\
10 & \quad (3,0,1/2,1/2,0) \quad x,1/4,0 \\
11 & \quad (3,0,1/2,2,1/2,0) \quad x,1/4,0 \\
12 & \quad (3,0,1/2,2,1/2,0) \quad x,1/4,0 \\
\end{align*}
Continued

(13) $\overline{1}$ 0,0,0
   (1) | 0,0,0)

(14) a (1/2,0,0) x,y,1/4
   (m$_z$ | 1/2,0,1/2)

(15) c (0,0,1/2) x,1/4,z
   (m$_y$ | 0,1/2,1/2)

(16) b (0,1/2,0) 1/4,y,z
   (m$_x$ | 1/2,1/2,0)

(17) $\overline{3}$ x,x,x;
   0,0,0
   (3$_{xyz}$ | 0,0,0)

(18) $\overline{3}$ x-1/2,x+1/2,x;
   1/2,1/2
   (3$_{xyz}^{-1}$ | 1/2,1/2,0)

(19) $\overline{3}$ x+1/2,x+1/2,x;
   1/2,1/2,0
   (3$_{xyz}^{-1}$ | 1/2,0,1/2)

(20) $\overline{3}$ x+1,x+1/2,x;
   1/2,0,1/2
   (3$_{xyz}^{-1}$ | 0,1/2,1/2)

(21) $\overline{3}$ x,x,x;
   0,0,0
   (3$_{xyz}^{-1}$ | 0,1/2,1/2)

For (1/2,1/2,1/2) + set

(1) 1
(1/2,1/2,1/2)

(2) 2 0,1/4,z
(2$_z$ | 0,1/2,0)

(3) 2 1/4,y,0
(2$_y$ | 1/2,0,0)

(4) 2 x,0,1/4
(2$_x$ | 0,0,1/2)

(5) $\overline{3}$ (1/2,1/2,1/2) x,x,x
   (3$_{xyz}$ | 1/2,1/2,1/2)

(6) $\overline{3}$ (1/6,-1/6,1/6)
   x-1/6,x+1/3,x
   (3$_{xyz}^{-1}$ | 0,0,1/2)

(7) $\overline{3}$ (-1/6,1/6,1/6)
   x+1/6,x+1/3,x
   (3$_{xyz}^{-1}$ | 0,1/2,0)

(8) $\overline{3}$ (1/6,1/6,-1/6)
   x+1/3,x+1/6,x
   (3$_{xyz}^{-1}$ | 1/2,0,0)

(9) $\overline{3}$ (1/2,1/2,1/2) x,x,x
   (3$_{xyz}^{-1}$ | 1/2,1/2,1/2)

(10) $\overline{3}$ (1/6,-1/6,-1/6)
   x+1/6,x+1/3,x
   (3$_{xyz} | 0,0,1/2)

(11) $\overline{3}$ (-1/6,1/6,-1/6)
   x+1/3,x+1/6,x
   (3$_{xyz} | 0,1/2,0)

(12) $\overline{3}$ (-1/6,1/6,1/6)
   x-1/6,x+1/3,x
   (3$_{xyz} | 0,0,1/2)

(13) $\overline{1}$ 1/4,1/4,1/4
   (1/2,1/2,1/2)

(14) b (0,1/2,0) x,y,0
   (m$_z$ | 0,1/2,0)

(15) a (1/2,0,0) x,0,z
   (m$_y$ | 1/2,0,0)

(16) c (0,0,1/2) 0,y,z
   (m$_x$ | 0,0,1/2)

(17) $\overline{3}$ x,x,x;
   1/4,1/4,1/4
   (3$_{xyz} | 1/2,1/2,1/2)

(18) $\overline{3}$ x-1/2,x,x;
   1/4,-1/4,1/4
   (3$_{xyz}^{-1}$ | 0,0,1/2)

(19) $\overline{3}$ x+1/2,x+1/2,x;
   1/4,-1/4,1/4
   (3$_{xyz}^{-1}$ | 0,1/2,0)

(20) $\overline{3}$ x+1/2,x,x;
   1/4,-1/4,1/4
   (3$_{xyz}^{-1}$ | 1/2,0,0)

(21) $\overline{3}$ x,x,x;
   1/4,1/4,1/4
   (3$_{xyz}^{-1} | 1/2,1/2,1/2)

(22) $\overline{3}$ x+1/2,x-1/2,x;
   1/4,-1/4,1/4
   (3$_{xyz}^{-1} | 0,0,1/2)

(23) $\overline{3}$ x,x+1/2,x;
   1/4,-1/4,1/4
   (3$_{xyz}^{-1} | 0,1/2,0)

(24) $\overline{3}$ x+1/2,x,x;
   1/4,-1/4,1/4
   (3$_{xyz}^{-1} | 1/2,0,0)

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity
Wyckoff letter
Site Symmetry.
24  d  2..  x,0,1/4 [u,0,0]  \( \bar{x}+1/2,0,3/4 [u,0,0] \)  \( \frac{1}{4},x,0 [0,u,0] \)  \( 3/4,\bar{x}+1/2,0 [0,\bar{u},0] \)  
    \( 0,1/4,x [0,0,u] \)  \( 0,3/4,\bar{x}+1/2 [0,0,\bar{u}] \)  \( \bar{x},0,3/4 [u,0,0] \)  \( x+1/2,0,1/4 [\bar{u},0,0] \)  
    \( 3/4,\bar{x},0 [0,u,0] \)  \( 1/4,\bar{x}+1/2,0 [0,u,0] \)  \( 0,3/4,\bar{x} [0,0,u] \)  \( 0,1/4,\bar{x}+1/2 [0,0,\bar{u}] \)  
16  c  .3.  x,x,x [u,u,u]  \( \bar{x}+1/2,x,x+1/2 [u,u,u] \)  \( \bar{x},x+1/2,x+1/2 [u,u,u] \)  \( x+1/2,\bar{x}+1/2,x [u,u,u] \)  
    \( \bar{x},\bar{x},\bar{x} [u,u,u] \)  \( x+1/2,\bar{x},\bar{x}+1/2 [u,u,u] \)  \( \bar{x},x+1/2,\bar{x}+1/2 [u,u,u] \)  \( \bar{x}+1/2,\bar{x}+1/2,x [u,u,u] \)  
8   b  .3.  1/4,1/4,1/4 [u,u,u]  \( 1/4,3/4,3/4 [u,u,u] \)  \( 3/4,3/4,1/4 [u,u,u] \)  \( 3/4,1/4,3/4 [u,u,u] \)  
8   a  .3.  0,0,0 [u,u,u]  \( 1/2,0,1/2 [u,u,u] \)  \( 0,1/2,1/2 [u,u,u] \)  \( 1/2,1/2,0 [u,u,u] \)  

**Symmetry of Special Projections**

Along [0,0,1]  \( p_{2\bar{y}} \)  2mm  
\( a^* = a/2 \)  \( b^* = b/2 \)  
Origin at 0,1/4,z

Along [1,1,1]  \( p6' \)  
\( a^* = (2a - b - c)/3 \)  \( b^* = (-a + 2b - c)/3 \)  
Origin at x,x,x

Along [1,1,0]  \( p2'mg' \)  
\( a^* = (-a + b)/2 \)  \( b^* = c/2 \)  
Origin at x,x,0
Origin at centre

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad z \leq \min (x,y) \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2 \]

Symmetry Operations

For \((0,0,0) + \) set

1. \(1 \quad (1') 0,0,0 \)
2. \(2 \quad (0,0,1/2) \quad 1/4,0,z \quad (2,1/2,0,1/2) \)
3. \(2 \quad (0,1/2,0) \quad 0,y,1/4 \quad (2,1/2,1/2,0) \)
4. \(2 \quad (1/2,0,0) \quad x,1/4,0 \)
5. \(3^+ x,x,x \quad (3_{xyz}^{0,0,0,0}) \)
6. \(3^- \quad \&+1/2,x,\& \quad (3_{xyz}^{-1/2,1/2,0}) \)
7. \(3^- \quad x+1/2,\&-1/2,\& \quad (3_{xyz}^{1/2,0,1/2}) \)
8. \(3^- \quad \&,\&+1/2,x \quad (3_{xyz}^{0,1/2,1/2}) \)
9. \(3^- x,x,x \quad (3_{xyz}^{-1/2,0,0,0}) \)
10. \(3^- (-1/3,1/3,1/3) \quad x+1/6,\&+1/6,\& \quad (3_{xyz}^{0,1/2,1/2}) \)
11. \(3^- (1/3,1/3,-1/3) \quad \&+1/3,\&+1/6,\& \quad (3_{xyz}^{0,1/2,1/2,0}) \)
12. \(3^- (1/3,-1/3,1/3) \quad \&-1/6,\&+1/3,\& \quad (3_{xyz}^{1/2,0,1/2}) \)
Continued 206.2.1539  la31'

For (1/2,1/2,1/2)' + set

(1) 1' (2) 2' 0,1/4,z (3) 2' 1/4,y,0 (4) 2' x,0,1/4
(1/2,1/2,1/2)' (2/2,1/2,0)' (2/2,1/2,0)' (2,0,1/2)'

(5) 3' · (1/2,1/2,1/2) x,x,x (6) 3' · (1/6,-1/6,1/6)
(3,xyz | 1/2,1/2,1/2) (3,xyz | 1/2,1/2,1/2)

(1) 1/2,1/2,1/2)' (2 0,1/2,0)' (2 y 1/2,0,0)'

(9) 3' · (1/2,1/2,1/2) x,x,x (10) 3' · (1/6,-1/6,1/6)
(3,xyz | 1/2,1/2,1/2)' (3,xyz | 1/2,1/2,1/2)'

(13) 3' · 1/4,1/4,1/4 (14) b' (0,1/2,0) x,y,0
(1/2,1/2,1/2)'

(17) 3' · x,x,x; (18) 3' · x-1/2,x, x;
(3,xyz | 1/2,1/2,1/2)' (3,xyz | 1/2,1/2,1/2)'

(21) 3' · x,x,x; (22) 3' · x+1/2,x-1/2,x;
(3,xyz | 1/2,1/2,1/2)' (3,xyz | 1/2,1/2,1/2)'

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z</td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>(5) z,x,y</td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>(9) y,z,x</td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>(13) x,y,z</td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>(17) z,x,y</td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>(21) y,z,x</td>
<td>(0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' +</td>
</tr>
</tbody>
</table>

24 d 2..1'

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) x+1/2,y,z+1/2</td>
<td>x+1/2,0,0</td>
</tr>
<tr>
<td>(6) z+1/2,y+1/2,x</td>
<td>z+1/2,0,0</td>
</tr>
<tr>
<td>(10) y,z+1/2,x+1/2</td>
<td>y+1/2,0,0</td>
</tr>
<tr>
<td>(14) x+1/2,y+1/2,z</td>
<td>x+1/2,0,0</td>
</tr>
<tr>
<td>(18) z+1/2,x+1/2,y</td>
<td>z+1/2,0,0</td>
</tr>
<tr>
<td>(22) y,z+1/2,x+1/2</td>
<td>y+1/2,0,0</td>
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</tbody>
</table>

206.2.1539 - 3 - 3436
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along</th>
<th>P2mm $1'$</th>
<th>P6 $1'$</th>
<th>P2mg $1'$</th>
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</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>$a^* = a/2$</td>
<td>$a^* = (2a - b - c)/3$</td>
<td>$a^* = (-a + b)/2$</td>
</tr>
<tr>
<td>[1,1,1]</td>
<td>$b^* = b/2$</td>
<td>$b^* = (-a + 2b - c)/3$</td>
<td>$b^* = c/2$</td>
</tr>
<tr>
<td>Origin</td>
<td>0,0,z</td>
<td>x,x,x</td>
<td>x,x,0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>b</th>
<th>.3 1'</th>
<th>1/4,1/4,1/4 [0,0,0]</th>
<th>1/4,3/4,3/4 [0,0,0]</th>
<th>3/4,3/4,1/4 [0,0,0]</th>
<th>3/4,1/4,3/4 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>a</td>
<td>.3 1'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Origin at center (3’)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; z ≤ min (x,y)

Vertices
0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/2,1/2,1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z
(2z | 1/2,0,1/2)

(3) 2 (0,1/2,0) 0,y,1/4
(2y | 0,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2z | 1/2,1/2,0)

(5) 3’ x,x,x
(3xyz | 0,0,0)

(6) 3’ x+1/2,x,x
(3xyz⁻¹ | 1/2,1/2,0)

(7) 3’ x+1/2, x-1/2,x
(3xyz⁻¹ | 1/2,0,1/2)

(8) 3’ x,x+1/2,x
(3xyz⁻¹ | 0,1/2,1/2)

(9) 3' x,x,x
(3xyz⁻¹ | 0,0,0)

(10) 3’ (-1/3,1/3,1/3)

x+1/6, x+1/6, x
(3xyz | 0,1/2,1/2)

(11) 3’ (1/3,1/3,-1/3)

x+1/3, x+1/6, x
(3xyz | 1/2,1/2,0)

(12) 3’ (1/3,-1/3,1/3)

x-1/6, x+1/3, x
(3xyz | 1/2,0,1/2)
(13) \( \overline{1} \cdot \begin{array}{c} 0,0,0 \\ 0,0,0' \end{array} \)
(14) \( a' \cdot \begin{array}{c} (1/2,0,0) \\ x,y,1/4 \\ m_x,1/2,0,1/2' \end{array} \)
(15) \( c' \cdot \begin{array}{c} (0,0,1/2) \\ x,1/4,z \\ m_y,0,1/2,1/2' \end{array} \)
(16) \( b' \cdot \begin{array}{c} (0,1/2,0) \\ 1/4,y,z \\ m_z,1/2,1/2,0' \end{array} \)

(17) \( 3^{+} \cdot \begin{array}{c} x,x,x; \\ 0,0,0' \end{array} \)
(18) \( 3^{+} \cdot \begin{array}{c} x+1/2,x+1,\bar{x}; \\ 0,1/2,1/2 \\ \bar{x} \end{array} \)
(19) \( 3^{+} \cdot \begin{array}{c} x+1/2,\bar{x}+1/2,x; \\ 1,2,1/2,0 \\ \bar{x}+1/2,0 \end{array} \)
(20) \( 3^{+} \cdot \begin{array}{c} x+1,\bar{x}+1/2,x; \\ 1/2,0,1/2 \\ \bar{x}+1/2,1/2,0 \end{array} \)

(21) \( 3^{+} \cdot \begin{array}{c} x,x,x; \\ 0,0,0 \\ \bar{x} \end{array} \)
(22) \( 3^{+} \cdot \begin{array}{c} x+1/2,\bar{x}-1/2,\bar{x}; \\ 0,0,1/2 \\ \bar{x} \end{array} \)
(23) \( 3^{+} \cdot \begin{array}{c} x+1/2,\bar{x},x; \\ 0,1/2,0 \\ \bar{x} \end{array} \)
(24) \( 3^{+} \cdot \begin{array}{c} x+1/2,\bar{x},x; \\ 1/2,0,0 \\ \bar{x} \end{array} \)

For \((1/2,1/2,1/2) + \) set

\[
\begin{array}{c}
(1) 1 \\
(1/2,1/2,1/2) \\
(2) 2 \cdot 0,1/4,0 \\
(2) 2 \cdot 1/4,0,0 \\
(5) 3^{+} \cdot (1/2,1/2,1/2) \quad x,x,x \\
(6) 3^{+} \cdot (1/6,-1/6,1/6) \quad x-1/6, x+1/3, x \\
(3_{xyz},1/2,1/2,1/2) \\
(7) 3^{+} \cdot (-1/6,1/6,1/6) \quad x+1/6, x+1/6, x \\
(3_{xyz},1/2,1/2,1/2) \\
(8) 3^{+} \cdot (1/6,1/6,-1/6) \quad x+1/3, x+1/6, x \\
(3_{xyz},1/2,1/2,1/2) \\
(9) 3^{+} \cdot (1/2,1/2,1/2) \quad x,x,x \\
(10) 3^{+} \cdot (1/6,-1/6,1/6) \quad x+1/6, x+1/6, x \\
(3_{xyz},1/2,1/2,1/2) \\
(11) 3^{+} \cdot (-1/6,1/6,1/6) \quad x+1/3, x+1/6, x \\
(3_{xyz},1/2,1/2,1/2) \\
(12) 3^{+} \cdot (-1/6,1/6,-1/6) \quad x+1/3, x+1/6, x \\
(3_{xyz},1/2,1/2,1/2) \\
(13) \overline{1} \cdot 1/4,1/4,1/4 \\
(1) 1/2,1/2,1/2' \\
(14) b' \cdot (0,1/2,0) \quad x,y,0 \\
(3_{xyz},1/2,1/2,1/2) \\
(15) a' \cdot (1/2,0,0) \quad x,0,z \\
(3_{xyz},1/2,1/2,1/2) \\
(16) c' \cdot (0,0,1/2) \quad 0,y,z \\
(3_{xyz},1/2,1/2,1/2) \\
(17) 3^{+} \cdot x,x,x; \\
(18) 3^{+} \cdot x-1/2,x,x; \\
(4,1/4,1/4,1/4) \\
(3_{xyz},1/2,1/2,1/2) \\
(19) 3^{+} \cdot x-1/2,\bar{x}+1/2,\bar{x}; \\
(1/4,-1/4,1/4) \\
(3_{xyz},1/2,1/2,1/2) \\
(20) 3^{+} \cdot \bar{x}-1/2,x;x; \\
(1/4,-1/4,-1/4) \\
(3_{xyz},1/2,1/2,1/2) \\
(21) 3^{+} \cdot x,x,x; \\
(22) 3^{+} \cdot x+1/2,\bar{x}-1/2,\bar{x}; \\
(4,1/4,1/4,1/4) \\
(3_{xyz},1/2,1/2,1/2) \\
(23) 3^{+} \cdot \bar{x}-1/2,x,x; \\
(1/4,-1/4,1/4) \\
(3_{xyz},1/2,1/2,1/2) \\
(24) 3^{+} \cdot \bar{x}-1/2,x,x; \\
(1/4,-1/4,-1/4) \\
(3_{xyz},1/2,1/2,1/2) \\
\end{array}
\]

Generators selected \( (1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13). \)

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>Wyckoff letter</td>
<td></td>
</tr>
<tr>
<td>Site Symmetry</td>
<td></td>
</tr>
<tr>
<td>48 e 1</td>
<td></td>
</tr>
</tbody>
</table>

\[\begin{array}{cccc}
(1) x,y,z [u,v,w] & (2) \bar{x}+1/2, \bar{y},z+1/2 [u,\bar{v},\bar{w}] & (3) \bar{x},y+1/2,\bar{z}+1/2 [\bar{u},\bar{v},\bar{w}] & (4) x+1/2, \bar{y}+1/2, z [u,v,w] \\
(5) x,z,y [w,u,v] & (6) z+1/2, \bar{x}+1/2, \bar{y} [w,\bar{u},\bar{v}] & (7) z+1/2, x,y+1/2 [\bar{w},u,v] & (8) \bar{z},x+1/2, \bar{y}+1/2 [w,u,v] \\
(9) y,z,x [v,w,u] & (10) \bar{y},z+1/2, x+1/2 [\bar{v},w,u] & (11) y+1/2, z+1/2, x [v,w,u] & (12) \bar{y}+1/2, z+1/2, x [\bar{v},w,u] \\
(13) \bar{x},y,z [u,\bar{v},\bar{w}] & (14) x+1/2, y,z+1/2 [u,v,\bar{w}] & (15) x,\bar{y}+1/2, z+1/2 [u,v,\bar{w}] & (16) x+1/2, y+1/2, z [\bar{u},v,\bar{w}] \\
(17) \bar{x},z,y [\bar{w},u,\bar{v}] & (18) \bar{z}+1/2,x+1/2, y [w,\bar{u},\bar{v}] & (19) z+1/2, \bar{y}, x+1/2 [w,u,v] & (20) z, x+1/2, y+1/2 [w,\bar{u},\bar{v}] \\
(21) \bar{y},z,x [\bar{v},w,u] & (22) y, \bar{z}+1/2,x+1/2 [\bar{v},w,u] & (23) \bar{y}+1/2, z+1/2, x [\bar{v},w,u] & (24) y+1/2, z+1/2, x [\bar{v},w,u] \\
\end{array}\]
Symmetry of Special Projections

Along [0,0,1] p2m'm'
\( a^* = a/2 \quad b^* = b/2 \)

Along [1,1,1] p6
\( a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \)

Along [1,1,0] p2m'g'
\( a^* = (-a + b)/2 \quad b^* = c/2 \)

Origin at 0,0,z
Origin at x,x,x
Origin at x,x,0

Ia'\bar{3}'

Cubic
Origin at center (3)

Asymmetric unit

\[ 0 < x < 1/2; \quad 0 < y < 1/2; \quad 0 < z < 1/2; \quad z < \min(x, y) \]

Vertices

\[ (0,0,0) \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/2,1/2,1/2 \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \(1\)
2. \(2 (0,0,1/2) \quad 1/4,0,z\)
3. \(2 (0,1/2,0) \quad 0,y,1/4\)
4. \(2 (1/2,0,0) \quad x,1/4,0\)

5. \(3^+ x,x,x\)
6. \(3^+ x+1/2,x,x\)
7. \(3^+ x+1/2,x-1/2,x\)
8. \(3^+ x,x+1/2,x\)

9. \(3^- x,x,x\)
10. \(3^- (-1/3,1/3,1/3) \quad x+1/6,x+1/6,x\)
11. \(3^- (1/3,1/3,-1/3) \quad x+1/3,x+1/3,x\)
12. \(3^- (1/3,-1/3,1/3) \quad x-1/6,x+1/3,x\)

Continued

206.4.1541

206.4.1541 - 2 - 3441
Continued 206.4.1541 - 3 - 3442

\[
\begin{align*}
(13) & \quad \bar{1} \ 0,0,0 \\
(14) & \quad a \ (1/2,0,0) \ x,y,1/4 \\
(15) & \quad c \ (0,0,1/2) \ x,1/4,z \\
(16) & \quad b \ (0,1/2,0) \ 1/4,y,z
\end{align*}
\]

\[
\begin{align*}
(17) & \quad 3^+ \ x,x,x; \\
(18) & \quad 3^+ \ x-1/2,x+1/2,x; \\
(19) & \quad 3^+ \ x+1/2,x+1/2,x; \\
(20) & \quad 3^+ \ x+1/2,x+1/2,x
\end{align*}
\]

\[
\begin{align*}
(21) & \quad 3^- \ x,x,x; \\
(22) & \quad 3^- \ x+1/2,x-1/2,x; \\
(23) & \quad 3^- \ x,x+1/2,x; \\
(24) & \quad 3^- \ x+1/2,x,x
\end{align*}
\]

For \((1/2,1/2,1/2)^+\) + set

\[
\begin{align*}
(1) & \quad 1' \\
(2) & \quad 2' \ 0,1/4,z \\
(3) & \quad 2' \ 1/4,y,0 \\
(4) & \quad 2' \ x,0,1/4
\end{align*}
\]

\[
\begin{align*}
(5) & \quad 3^+ \ (1/2,1/2,1/2) \ x,x,x \\
(6) & \quad 3^+ \ (1/6,-1/6,1/6) \ x-1/6,x+1/3,x \\
(7) & \quad 3^+ \ (1/6,-1/6,1/6) \ x+1/6,x+1/6,x \\
(8) & \quad 3^+ \ (1/6,1/6,-1/6) \ x+1/3,x+1/6,x
\end{align*}
\]

\[
\begin{align*}
(9) & \quad 3^- \ (1/2,1/2,1/2) \ x,x,x \\
(10) & \quad 3^- \ (1/6,-1/6,1/6) \ x+1/6,x+1/6,x \\
(11) & \quad 3^- \ (1/6,-1/6,1/6) \ x+1/3,x+1/6,x \\
(12) & \quad 3^- \ (1/6,1/6,-1/6) \ x+1/3,x+1/6,x
\end{align*}
\]

\[
\begin{align*}
(13) & \quad \bar{1}^- \ 1/4,1/4,1/4 \\
(14) & \quad b' \ (0,1/2,0) \ x,y,0 \\
(15) & \quad a' \ (1/2,0,0) \ x,0,z \\
(16) & \quad c' \ (0,0,1/2) \ 0,y,z
\end{align*}
\]

\[
\begin{align*}
(17) & \quad 3^+ \ x,x; \\
(18) & \quad 3^+ \ x-1/2,x-1/2,x \\
(19) & \quad 3^+ \ x-1/2,x+1/2,x \\
(20) & \quad 3^+ \ x,x-1/2,x
\end{align*}
\]

\[
\begin{align*}
(21) & \quad 3^- \ x,x,x; \\
(22) & \quad 3^- \ x+1/2,x-1/2,x; \\
(23) & \quad 3^- \ x,x+1/2,x; \\
(24) & \quad 3^- \ x+1/2,x,x
\end{align*}
\]

Generators selected \((1): t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).\)

Positions

\[
\begin{align*}
\text{Multiplicity,} \\
\text{Wyckoff letter,} \\
\text{Site Symmetry.}
\end{align*}
\]

\[
\begin{align*}
&\text{Coordinates} \\
&\ (0,0,0) + (1/2,1/2,1/2)^+ \\
&\ (1) \ x,y,z \ [u,v,w] \\
&\ (2) \ x+1/2,y,z+1/2 \ [u,v,w] \\
&\ (3) \ x,y+1/2,z+1/2 \ [u,v,w] \\
&\ (4) \ x+1/2,y+1/2,z \ [u,v,w]
\end{align*}
\]

\[
\begin{align*}
&\ (5) \ z,x,y \ [w,u,v] \\
&\ (6) \ z+1/2,x+1/2,y \ [w,u,v] \\
&\ (7) \ z+1/2,x,y+1/2 \ [w,u,v] \\
&\ (8) \ z,x+1/2,y+1/2 \ [w,u,v]
\end{align*}
\]

\[
\begin{align*}
&\ (9) \ y,z,x \ [v,w,u] \\
&\ (10) \ y,z+1/2,x+1/2 \ [v,w,u] \\
&\ (11) \ y+1/2,z+1/2,x \ [v,w,u] \\
&\ (12) \ y+1/2,z,x+1/2 \ [v,w,u]
\end{align*}
\]

\[
\begin{align*}
&\ (13) \ x,y,z \ [u,v,w] \\
&\ (14) \ x+1/2,y,z+1/2 \ [u,v,w] \\
&\ (15) \ x,y+1/2,z+1/2 \ [u,v,w] \\
&\ (16) \ x+1/2,y+1/2,z \ [u,v,w]
\end{align*}
\]

\[
\begin{align*}
&\ (17) \ z,x,y \ [w,u,v] \\
&\ (18) \ z+1/2,x+1/2,y \ [w,u,v] \\
&\ (19) \ z+1/2,x,y+1/2 \ [w,u,v] \\
&\ (20) \ z,x+1/2,y+1/2 \ [w,u,v]
\end{align*}
\]

\[
\begin{align*}
&\ (21) \ y,z,x \ [v,w,u] \\
&\ (22) \ y,z+1/2,x+1/2 \ [v,w,u] \\
&\ (23) \ y+1/2,z+1/2,x \ [v,w,u] \\
&\ (24) \ y+1/2,z,x+1/2 \ [v,w,u]
\end{align*}
\]\n
Continued 206.4.1541 \(I_b, a\bar{a}\)
Symmetry of Special Projections

Along [0,0,1] \(p_{2a}\) 2mm
\[a^* = \frac{b}{2}, \quad b^* = -\frac{a}{2}\]
Origin at 0,0,z

Along [1,1,1] \(p61'\)
\[a^* = \frac{(2a - b - c)}{3}, \quad b^* = \frac{(-a + 2b - c)}{3}\]
Origin at x,x,x

Along [1,1,0] \(p_{2a}\) 2mg
\[a^* = \frac{(-a + b)}{2}, \quad b^* = \frac{c}{2}\]
Origin at x,x,0
Origin at 432

Asymmetric unit:

\begin{align*}
0 &\leq x \leq 1; \\
0 &\leq y \leq 1/2; \\
0 &\leq z \leq 1/2; \\
y &\leq \min(x,1-x); \\
z &\leq y
\end{align*}

Vertices:

\begin{align*}
0,0,0 &\quad 1,0,0 &\quad 1/2,1/2,0 &\quad 1/2,1/2,1/2
\end{align*}

Symmetry Operations:

\begin{align*}
(1) &\quad 1 \\
&\quad (1|0,0,0) \\
(2) &\quad 2,0,0,z \\
&\quad (2z|0,0,0) \\
(3) &\quad 2,0,y,0 \\
&\quad (2y|0,0,0) \\
(4) &\quad 2,x,0,0 \\
&\quad (2z|0,0,0) \\
(5) &\quad 3^+ x,x,x \\
&\quad (3xyz|0,0,0) \\
(6) &\quad 3^+ x,x,x \\
&\quad (3_{xyz}^{-1}|0,0,0) \\
(7) &\quad 3^+ x,x,x \\
&\quad (3_{xyz}^{-1}|0,0,0) \\
(8) &\quad 3^+ x,x,x \\
&\quad (3_{xyz}^{-1}|0,0,0) \\
(9) &\quad 3^- x,x,x \\
&\quad (3_{xyz}^{-1}|0,0,0) \\
(10) &\quad 3^- x,x,x \\
&\quad (3_{xyz}^{-1}|0,0,0) \\
(11) &\quad 3^- x,x,x \\
&\quad (3_{xyz}^{-1}|0,0,0) \\
(12) &\quad 3^- x,x,x \\
&\quad (3_{xyz}^{-1}|0,0,0)
\end{align*}
Continued

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 k 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(3) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(5) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(6) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(7) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(8) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(9) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(10) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(11) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(12) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(13) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(14) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(15) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(16) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(17) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(18) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(19) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(20) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(21) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(22) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(23) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(24) x,y,z [u,v,w]</td>
</tr>
</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Site Symmetry.

207.1.1542  P432
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along</th>
<th>p4m'</th>
<th>[0,1,1]</th>
<th>p3m'1</th>
<th>[1,1,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td>a*</td>
<td>a</td>
<td>a* = (2a - b - c)/3</td>
<td>b*</td>
<td>(-a + 2b - c)/3</td>
</tr>
<tr>
<td>b*</td>
<td>b</td>
<td>(-a + b)/2</td>
<td>c</td>
<td>c</td>
</tr>
<tr>
<td>a</td>
<td>a</td>
<td>(2a - b - c)/3</td>
<td>b</td>
<td>(-a + 2b - c)/3</td>
</tr>
<tr>
<td>b</td>
<td>b</td>
<td>(-a + b)/2</td>
<td>c</td>
<td>c</td>
</tr>
</tbody>
</table>

Origin at 0,0,z

Origin at x,x,x

Origin at x,x,0
Origin at 4321′

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad y \leq \min(x, 1-x); \quad z \leq y \]

Vertices

\[ 0,0,0 \quad 1,0,0 \quad \frac{1}{2},1/2,0 \quad 1/2,1/2,1/2 \]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad (0,0,0) \\
(2) & \quad (0,0,z) \\
(3) & \quad (0,y,0) \\
(3) & \quad (2,0,0,0) \\
(4) & \quad (2,0,0,0) \\
(5) & \quad (0,0,0) \\
(5) & \quad (0,0,0) \\
(6) & \quad (0,0,0) \\
(6) & \quad (0,0,0) \\
(7) & \quad (0,0,0) \\
(7) & \quad (2,0,0,0) \\
(8) & \quad (2,0,0,0) \\
(8) & \quad (2,0,0,0) \\
(9) & \quad (0,0,0) \\
(9) & \quad (0,0,0) \\
(10) & \quad (0,0,0) \\
(10) & \quad (0,0,0) \\
(11) & \quad (0,0,0) \\
(11) & \quad (0,0,0) \\
(12) & \quad (0,0,0) \\
(12) & \quad (0,0,0) \\
\end{align*}
\]
Continued

(13) 2 \ x,x,0
    (14) 2 \ x,-x,0
    (15) 4' \ 0,0,z
    (16) 4' \ 0,0,z
    (2xy \ 0,0,0)
    (2xy \ 0,0,0)
    (4z \ 0,0,0)
    (4z \ 0,0,0)

(17) 4' \ x,0,0
    (18) 2 \ 0,y,y
    (19) 2 \ 0,y,-y
    (20) 4' \ x,0,0
    (4x \ 0,0,0)
    (2yz \ 0,0,0)
    (2yz \ 0,0,0)

(21) 4' \ 0,y,0
    (22) 2 \ x,0,x
    (23) 4' \ 0,y,0
    (24) 2 \ x,0,x
    (4y \ 0,0,0)
    (2xz \ 0,0,0)
    (4y \ 0,0,0)

For 1' + set

(1) 1'
(1) 0,0,0
(2) 2' \ 0,0,z
    (2) 0,0,0
(3) 2' \ 0,y,y
    (3) 0,0,0
(4) 2' \ x,0,0
    (4) 0,0,0

(5) 3'
(3) x,x,x
(3) 0,0,0
(6) 3' \ x,-x,-x
    (3) 0,0,0
(7) 3' \ x,x,-x
    (3) 0,0,0
(8) 3' \ x,-x,-x
    (3) 0,0,0

(9) 3' \ x,x,x
(3) 0,0,0
(10) 3' \ x,-x,-x
    (3) 0,0,0
(11) 3' \ x,x,-x
    (3) 0,0,0
(12) 3' \ x,-x,-x
    (3) 0,0,0

(13) 2' \ x,0,0
    (2) x,0,0
(14) 2' \ x,-x,0
    (2) x,0,0
(15) 4' \ 0,0,z
    (4) z \ 0,0,0
(16) 4' \ 0,0,z
    (4) z \ 0,0,0

(17) 4' \ x,0,0
    (4) x \ 0,0,0
(18) 2' \ 0,y,y
    (2) y \ 0,0,0
(19) 2' \ 0,y,-y
    (2) y \ 0,0,0
(20) 4' \ x,0,0
    (4) y \ 0,0,0

(21) 4' \ 0,y,0
    (4) y \ 0,0,0
(22) 2' \ x,0,x
    (2) x \ 0,0,0
(23) 4' \ 0,y,0
    (4) z \ 0,0,0
(24) 2' \ x,0,x
    (2) x \ 0,0,0

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

24 k 11'

(1) x,y,z [0,0,0]
(2) \ x,y,-z [0,0,0]
(3) \ x,y,z [0,0,0]
(4) x,y,-z [0,0,0]

(5) z,x,y [0,0,0]
(6) z,-x,-y [0,0,0]
(7) z,-x,y [0,0,0]
(8) z,x,-y [0,0,0]

(9) y,z,x [0,0,0]
(10) y,z,-x [0,0,0]
(11) y,z,x [0,0,0]
(12) y,z,-x [0,0,0]

(13) y,x,z [0,0,0]
(14) y,-x,z [0,0,0]
(15) y,x,z [0,0,0]
(16) y,-x,z [0,0,0]

(17) x,z,y [0,0,0]
(18) x,-z,y [0,0,0]
(19) x,z,y [0,0,0]
(20) x,-z,y [0,0,0]

(21) z,y,x [0,0,0]
(22) z,-y,x [0,0,0]
(23) z,y,x [0,0,0]
(24) z,-y,x [0,0,0]

12 j .21'
1/2,y,y [0,0,0]
1/2,y,y [0,0,0]
1/2,y,y [0,0,0]
1/2,y,y [0,0,0]

y,1/2,y [0,0,0]
y,1/2,y [0,0,0]
y,1/2,y [0,0,0]
y,1/2,y [0,0,0]

y,y,1/2 [0,0,0]
y,y,1/2 [0,0,0]
y,y,1/2 [0,0,0]
y,y,1/2 [0,0,0]
Symmetry of Special Projections

| 12 | i | .21' | 0,y,y [0,0,0] | 0,y,y [0,0,0] | 0,y,y [0,0,0] |
| 12 | h | 2.1' | x,1/2,0 [0,0,0] | 0,x,1/2 [0,0,0] | 0,x,1/2 [0,0,0] |
| 12 | f | 4.1' | x,1/2,1/2 [0,0,0] | 1/2,x,1/2 [0,0,0] |
| 8 | g | .3.1' | x,x,x [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |
| 6 | f | 4.1' | x,0,0 [0,0,0] | 0,x,0 [0,0,0] |
| 6 | e | 4.1' | 0,x,0 [0,0,0] | 0,0,x [0,0,0] |
| 3 | d | 42.21' | 1/2,0,0 [0,0,0] | 0,0,1/2 [0,0,0] |
| 3 | c | 42.21' | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |
| 1 | b | 4321' | 1/2,1/2,1/2 [0,0,0] |
| 1 | a | 4321' | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

- **Along [0,0,1]** p4mm1'
  - \(a^* = a\) \(b^* = b\)

- **Along [1,1,1]** p3m11'
  - \(a^* = \frac{2a - b - c}{3}\) \(b^* = \frac{-a + 2b - c}{3}\)

- **Along [1,1,0]** p2mm1'
  - \(a^* = \frac{-a + b}{2}\) \(b^* = c\)

**Origin at**
- 0,0,z
- x,x,x
- x,x,0
Origin at 4'32'

Asymmetric unit:
- \(0 \leq x \leq 1\)
- \(0 \leq y \leq \frac{1}{2}\)
- \(0 \leq z \leq \frac{1}{2}\)
- \(y \leq \min(x,1-x)\)
- \(z \leq y\)

Vertices:
- \(0,0,0\)
- \(1,0,0\)
- \(\frac{1}{2},\frac{1}{2},0\)
- \(\frac{1}{2},\frac{1}{2},\frac{1}{2}\)

Symmetry Operations:

1. \(1\)
   - \((1|0,0,0)\)

2. \(2\ 0,0,z\)
   - \((2z|0,0,0)\)

3. \(2\ 0,y,0\)
   - \((2y|0,0,0)\)

4. \(2\ x,0,0\)
   - \((2x|0,0,0)\)

5. \(3^+\ x,x,x\)
   - \((3_{xyz}|0,0,0)\)

6. \(3^+\ x,x,x\)
   - \((3_{xyz}^{-1}|0,0,0)\)

7. \(3^+\ x,x,x\)
   - \((3_{xyz}^{-1}|0,0,0)\)

8. \(3^+\ x,x,x\)
   - \((3_{xyz}^{-1}|0,0,0)\)

9. \(3^-\ x,x,x\)
   - \((3_{xyz}|0,0,0)\)

10. \(3^-\ x,x,x\)
    - \((3_{xyz}|0,0,0)\)

11. \(3^-\ x,x,x\)
    - \((3_{xyz}|0,0,0)\)

12. \(3^-\ x,x,x\)
    - \((3_{xyz}|0,0,0)\)
Continued

<table>
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<tr>
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<th>$2'$</th>
<th>$x, x, 0$</th>
<th>(14)</th>
<th>$2'$</th>
<th>$x, x, 0$</th>
<th>(15)</th>
<th>$4'$</th>
<th>$0, 0, z$</th>
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<th>$0, 0, z$</th>
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<tr>
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<td>0, 0, 0</td>
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<td>$0, y, y$</td>
<td>(20)</td>
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<td>($4_{y}$)</td>
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<td>($2_{yz}$)</td>
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<td>($2_{yz}$)</td>
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<td>$x, 0, x$</td>
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<td>$4'$</td>
<td>$0, y, 0$</td>
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<td>$</td>
<td>0, 0, 0</td>
<td>$</td>
<td></td>
<td>($2_{xz}$)</td>
<td>$</td>
<td>0, 0, 0</td>
<td>$</td>
<td></td>
<td>($4_{y}$)</td>
</tr>
</tbody>
</table>

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

**Positions**

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>24</th>
<th>k</th>
<th>1</th>
</tr>
</thead>
</table>

| (1) | $x, y, z$ | [u,v,w] |
| (5) | $z, x, y$ | [w,u,v] |
| (9) | $y, z, x$ | [v,w,u] |
| (13) | $y, x, z$ | [v,u,w] |
| (17) | $x, z, y$ | [u,w,v] |
| (21) | $z, y, x$ | [w,v,u] |

<table>
<thead>
<tr>
<th>12</th>
<th>j</th>
<th>..$2'$</th>
</tr>
</thead>
</table>

| (2) | $x, y, z$ | [u,v,w] |
| (3) | $x, y, z$ | [u,v,w] |
| (4) | $x, y, z$ | [u,v,w] |

<table>
<thead>
<tr>
<th>12</th>
<th>i</th>
<th>..$2'$</th>
</tr>
</thead>
</table>

| (6) | $z, x, y$ | [w,u,v] |
| (7) | $z, x, y$ | [w,u,v] |
| (8) | $z, x, y$ | [w,u,v] |

<table>
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<th>h</th>
<th>2..</th>
</tr>
</thead>
</table>

| (10) | $y, z, x$ | [v,w,u] |
| (11) | $y, z, x$ | [v,w,u] |
| (12) | $y, z, x$ | [v,w,u] |

<table>
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<th>8</th>
<th>g</th>
<th>..$3.$</th>
</tr>
</thead>
</table>

| (12) | $y, 0, y$ | [v,w,u] |
| (13) | $y, 0, y$ | [v,w,u] |
| (14) | $y, 0, y$ | [v,w,u] |

<table>
<thead>
<tr>
<th>6</th>
<th>f</th>
<th>4$'$.</th>
</tr>
</thead>
</table>

| (15) | $2$, $1/2, 0$ | [0,0,0] |
| (16) | $2$, $1/2, 0$ | [0,0,0] |
| (17) | $2$, $1/2, 0$ | [0,0,0] |

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Symmetry of Special Projections

Along [0,0,1]  p4'm'm
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,1,1]  p3m1
\[ a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \]
Origin at x,x,x

Along [1,1,0]  p2m'm'
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,0
Origin at 432

Asymmetric unit

\[ 0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min(x,1-x); \quad z \leq y \]

Vertices

- 0,0,0
- 1,0,0
- 1/2,1/2,0
- 1/2,1/2,1/2

Symmetry Operations

For (0,0,0) + set

1. \(1\)  
   \((1|0,0,0)\)

2. \(2\) 0,0,z  
   \((2_z|0,0,0)\)

3. \(2\) 0,y,0  
   \((2_y|0,0,0)\)

4. \(2\) x,0,0  
   \((2_x|0,0,0)\)

5. \(3^+\) x,x,x  
   \((3_{xyz}|0,0,0)\)

6. \(3^+\) x,x,x  
   \((3_{xyz}^{-1}|0,0,0)\)

7. \(3^+\) x,x,x  
   \((3_{xyz}^{-1}|0,0,0)\)

8. \(3^+\) x,x,x  
   \((3_{xyz}^{-1}|0,0,0)\)

9. \(3^-\) x,x,x  
   \((3_{xyz}^{-1}|0,0,0)\)

10. \(3^-\) x,x,x  
    \((3_{xyz}|0,0,0)\)

11. \(3^-\) x,x,x  
    \((3_{xyz}|0,0,0)\)

12. \(3^-\) x,x,x  
    \((3_{xyz}|0,0,0)\)
Continued

For $(1,0,0)\,^+$ set

(1) $t\,^+ (1,0,0)$
(1) $t\,(1,0,0)$
(1) $t\,(1,0,0)$'
(1) $t\,^+ (1,0,0)$

(2) $2\,^+ 1/2,0,z$
(2) $2\,^+ 1/2,0,z$
(2) $2\,^+ 1/2,0,z$
(2) $2\,^+ 1/2,0,z$

(3) $2\,^+ 1/2,y,0$
(3) $2\,^+ 1/2,y,0$
(3) $2\,^+ 1/2,y,0$
(3) $2\,^+ 1/2,y,0$

(4) $2\,^+ (1,0,0)$
(4) $2\,^+ (1,0,0)$
(4) $2\,^+ (1,0,0)$
(4) $2\,^+ (1,0,0)$

Generators selected

(1); $t\,^+ (1,0,0)$; $t\,(0,1,0)$; $t\,(0,0,1)$; (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48 k 1

(1) $x,y,z \,[u,v,w]$ (2) $\bar{x},\bar{y},z \,[\bar{u},\bar{v},\bar{w}]$ (3) $x,y,z \,[u,v,w]$ (4) $x,y,z \,[u,v,w]$

(5) $z,x,y \,[w,u,v]$ (6) $\bar{z},\bar{x},\bar{y} \,[\bar{w},\bar{u},\bar{v}]$ (7) $z,x,y \,[w,u,v]$ (8) $z,x,y \,[w,u,v]$

(9) $y,z,x \,[v,w,u]$ (10) $\bar{y},\bar{z},x \,[\bar{v},\bar{w},\bar{u}]$ (11) $y,z,x \,[v,w,u]$ (12) $y,z,x \,[v,w,u]$

(13) $y,x,z \,[v,u,w]$ (14) $\bar{y},\bar{x},\bar{z} \,[\bar{v},\bar{u},\bar{w}]$ (15) $y,z,x \,[v,u,w]$ (16) $y,z,x \,[v,u,w]$

(17) $x,z,y \,[u,w,v]$ (18) $\bar{x},\bar{z},\bar{y} \,[\bar{u},\bar{w},\bar{v}]$ (19) $x,z,y \,[u,w,v]$ (20) $x,z,y \,[u,w,v]$

(21) $z,y,x \,[w,v,u]$ (22) $\bar{z},\bar{y},\bar{x} \,[\bar{w},\bar{v},\bar{u}]$ (23) $z,y,x \,[w,v,u]$ (24) $z,y,x \,[w,v,u]$

(0,0,0) + (1,0,0) +
| 24 | j | 0.2' | 1/2,y,y [u,v,v] | 1/2,y,y [u,v,v] | 1/2,y,y [u,v,v] | 1/2,y,y [u,v,v] |
| 24 | i | 0.2 | 0,y,y [0,v,v] | 0,y,y [0,v,v] | 0,y,y [0,v,v] | 0,y,y [0,v,v] |
| 24 | h | 2'.. | x,1/2,0 [0,v,w] | x,1/2,0 [0,v,w] | 0,x,1/2 [w,0,v] | 0,x,1/2 [w,0,v] |
| 16 | g | .3 | x,x,x [u,u,u] | x,x,x [u,u,u] | x,x,x [u,u,u] | x,x,x [u,u,u] |
| 12 | f | 4'.. | x,1/2,1/2 [0,0,0] | 1/2,x,1/2 [0,0,0] | 1/2,x,1/2 [0,0,0] | 1/2,x,1/2 [0,0,0] |
| 12 | e | 4'.. | x,0,0 [u,0,0] | 0,x,0 [u,0,0] | 0,x,0 [u,0,0] | 0,x,0 [u,0,0] |
| 6  | d | 42'.2' | 1/2,0,0 [u,0,0] | 0,1/2,0 [u,0,0] | 0,1/2,0 [u,0,0] | 0,1/2,0 [u,0,0] |
| 6  | c | 4'2'.2 | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] |
| 2  | b | 4'32' | 1/2,1/2,1/2 [0,0,0] |
| 2  | a | 432' | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
<th>Along [1,1,0]</th>
<th>p3m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (2a - b - c)/3</td>
<td>b* = (-a + 2b - c)/3</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td>Origin at x,x,x</td>
<td></td>
</tr>
</tbody>
</table>
Origin at 23

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad -\frac{1}{4} \leq z \leq \frac{1}{4}; \quad \max (-x,x-\frac{1}{2},-y,y-\frac{1}{2}) \leq z \leq \min (x,1/2-x,y,1/2-y) \]

Vertices
\[ 0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4 \]

Symmetry Operations

(1) 1
\[ (1|0,0,0) \]

(2) 2, 0,0,z
\[ (2_z|0,0,0) \]

(3) 2, 0, y,0
\[ (2_y|0,0,0) \]

(4) 2, x, 0,0
\[ (2_x|0,0,0) \]

(5) 3, x,x, x
\[ (3_{xyz}|0,0,0) \]

(6) 3', x,x, x
\[ (3_{xyz}^{-1}|0,0,0) \]

(7) 3', x,x, x
\[ (3_{xyz}^{-1}|0,0,0) \]

(8) 3', x,x, x
\[ (3_{xyz}^{-1}|0,0,0) \]

(9) 3', x,x, x
\[ (3_{xyz}^{-1}|0,0,0) \]

(10) 3', x,x, x
\[ (3_{xyz}^{-1}|0,0,0) \]

(11) 3', x,x, x
\[ (3_{xyz}^{-1}|0,0,0) \]

(12) 3', x,x, x
\[ (3_{xyz}^{-1}|0,0,0) \]
Continued

<table>
<thead>
<tr>
<th>Number</th>
<th>Coordinates</th>
<th>Site Symmetry</th>
<th>Multiplicity</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>( z, x, y ) ( (2_{xy}) )</td>
<td>1/2,1/2,1/2</td>
<td>2</td>
<td>(13) ( (1/2,1/2,0) ) ( x, x, 1/4 ) ( (2_{xy}) )</td>
</tr>
<tr>
<td>14</td>
<td>( x, \bar{x} + 1/2, 1/4 ) ( (2_{xy}) )</td>
<td>1/2,1/2,1/2</td>
<td>2</td>
<td>(14) ( (2_{xy}) )</td>
</tr>
<tr>
<td>15</td>
<td>( 4^* ) ( (0,0,1/2) ) ( 1/2,0, z ) ( (4_{z}) )</td>
<td>1/2,1/2,1/2</td>
<td>1</td>
<td>(15) ( 4^* ) ( (0,0,1/2) ) ( 1/2,0, z ) ( (4_{z}) )</td>
</tr>
<tr>
<td>16</td>
<td>( 4^* ) ( (0,0,1/2) ) ( 0,1/2, z ) ( (4_{z}) )</td>
<td>1/2,1/2,1/2</td>
<td>1</td>
<td>(16) ( 4^* ) ( (0,0,1/2) ) ( 0,1/2, z ) ( (4_{z}) )</td>
</tr>
<tr>
<td>17</td>
<td>( 4^* ) ( (1/2,0,0) ) ( x, 1/2,0 ) ( (4_{x}) )</td>
<td>1/2,1/2,1/2</td>
<td>1</td>
<td>(17) ( 4^* ) ( (1/2,0,0) ) ( x, 1/2,0 ) ( (4_{x}) )</td>
</tr>
<tr>
<td>18</td>
<td>( 2 (0,1/2,1/2) ) ( 1/4, y, y ) ( (2_{yz}) )</td>
<td>1/2,1/2,1/2</td>
<td>2</td>
<td>(18) ( 2 (0,1/2,1/2) ) ( 1/4, y, y ) ( (2_{yz}) )</td>
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<tr>
<td>19</td>
<td>( 1/4, y + 1/2, y ) ( (2_{yz}) )</td>
<td>1/2,1/2,1/2</td>
<td>1</td>
<td>(19) ( 1/4, y + 1/2, y ) ( (2_{yz}) )</td>
</tr>
<tr>
<td>20</td>
<td>( 4^* ) ( (1/2,0,0) ) ( x, 0,1/2 ) ( (4_{x}) )</td>
<td>1/2,1/2,1/2</td>
<td>1</td>
<td>(20) ( 4^* ) ( (1/2,0,0) ) ( x, 0,1/2 ) ( (4_{x}) )</td>
</tr>
<tr>
<td>21</td>
<td>( 4^* ) ( (0,1/2,0) ) ( 1/2, y, 0 ) ( (4_{y}) )</td>
<td>1/2,1/2,1/2</td>
<td>1</td>
<td>(21) ( 4^* ) ( (0,1/2,0) ) ( 1/2, y, 0 ) ( (4_{y}) )</td>
</tr>
<tr>
<td>22</td>
<td>( 2 (1/2,0,1/2) ) ( x, 1/4, x ) ( (2_{xz}) )</td>
<td>1/2,1/2,1/2</td>
<td>2</td>
<td>(22) ( 2 (1/2,0,1/2) ) ( x, 1/4, x ) ( (2_{xz}) )</td>
</tr>
</tbody>
</table>

Generators selected

1; \( t(1,0,0) \); \( t(0,1,0) \); \( t(0,0,1) \); (2); (3); (5); (13).

Coordinates

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Site Symmetry</th>
<th>Wyckoff letter</th>
<th>12</th>
<th>14</th>
<th>16</th>
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<th>19</th>
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<tr>
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<td>[u,v,w]</td>
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<td>2</td>
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<td>6</td>
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<tr>
<td>2</td>
<td>( x, y, z )</td>
<td>[u,v,w]</td>
<td>1</td>
<td>2</td>
<td>3</td>
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<td>5</td>
<td>6</td>
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<tr>
<td>3</td>
<td>( x, y, z )</td>
<td>[u,v,w]</td>
<td>1</td>
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<tr>
<td>4</td>
<td>( x, y, z )</td>
<td>[u,v,w]</td>
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<td>[w,u,v]</td>
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<td>( z, x, y )</td>
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<td>( y+1/2, x+1/2, \bar{z}+1/2 )</td>
<td>[v,u,w]</td>
<td>(14) ( y+1/2, x+1/2, \bar{z}+1/2 )</td>
<td>[v,u,w]</td>
<td>(15) ( y+1/2, x+1/2, \bar{z}+1/2 )</td>
<td>[v,u,w]</td>
<td>(16) ( y+1/2, x+1/2, \bar{z}+1/2 )</td>
<td>[v,u,w]</td>
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<tr>
<td>( x+1/2, z+1/2, y+1/2 )</td>
<td>[u,w,v]</td>
<td>(17) ( x+1/2, z+1/2, y+1/2 )</td>
<td>[u,w,v]</td>
<td></td>
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<tr>
<td>( z+1/2, x+1/2, y+1/2 )</td>
<td>[w,v,u]</td>
<td>(21) ( z+1/2, x+1/2, y+1/2 )</td>
<td>[w,v,u]</td>
<td>(23) ( z+1/2, y+1/2, x+1/2 )</td>
<td>[w,v,u]</td>
<td>(24) ( z+1/2, y+1/2, x+1/2 )</td>
<td>[w,v,u]</td>
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<td>0,0,x [0,0,u]</td>
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<th>1/4,1/4,3/4 [0,0,0]</th>
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<td>3/4,3/4,1/4 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
<td>1/4,3/4,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

| 2  | a  | 23.  | 0,0,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |

Symmetry of Special Projections

Along [0,0,1] p4m\'m' \[a^* = a, \ b^* = b\] Along [1,1,1] p3m'1 \[a^* = (2a - b - c)/3, \ b^* = (-a + 2b - c)/3\] Along [1,1,0] p2m'1 \[a^* = (-a + b)/2, \ b^* = c\]
Origin at 231°

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; -1/4 ≤ z ≤ 1/4; max (-x,x-1/2,-y,y-1/2) ≤ z ≤ min (x,1/2-x,y,1/2-y)

Vertices: 0,0,0; 1/2,0,0; 1/2,1/2,0; 0,1/2,0; 1/4,1/4,1/4; 1/4,1/4,-1/4

Symmetry Operations

For 1 + set

(1) 1
(1 0 0 0)

(2) 2 0 0 z
(2 z 0 0 0)

(3) 2 0 y 0
(2 0 y 0 0)

(4) 2 x 0 0
(2 z 0 0 0)

(5) 3^* x x x
(3_{xyz} 0 0 0)

(6) 3^* x x x
(3_{xyz}^{-1} 0 0 0)

(7) 3^* x x x
(3_{xyz}^{-1} 0 0 0)

(8) 3^* x x x
(3_{xyz}^{-1} 0 0 0)

(9) 3^* x x x
(3_{xyz}^{-1} 0 0 0)

(10) 3^* x x x
(3_{xyz} 0 0 0)

(11) 3^* x x x
(3_{xyz} 0 0 0)

(12) 3^* x x x
(3_{xyz} 0 0 0)
Continued

(13) 2 (1/2,1/2,0) x,x,1/4
(2xy| 1/2,1/2,1/2)

(14) 2 x,x+1/2,1/4
(2xy| 1/2,1/2,1/2)

(15) 4' (0,0,1/2) 1/2,0,z
(4z^-1| 1/2,1/2,1/2)

(16) 4' (0,0,1/2) 0,1/2,z
(4z| 1/2,1/2,1/2)

(17) 4' (1/2,0,0) x,1/2,0
(4x^-1| 1/2,1/2,1/2)

(18) 2 (0,1/2,1/2) 1/4,y,y
(2yz| 1/2,1/2,1/2)

(19) 2 1/4,y+1/2,y
(2yz| 1/2,1/2,1/2)

(20) 4' (1/2,0,0) x,0,1/2
(4x| 1/2,1/2,1/2)

(21) 4' (0,1/2,0) 1/2,y,0
(4y| 1/2,1/2,1/2)

(22) 2 (1/2,0,1/2) x,1/4,x
(2xz| 1/2,1/2,1/2)

(23) 4' (0,1/2,0) 0,y,1/2
(4y^-1| 1/2,1/2,1/2)

(24) 2 x,x+1/2,1/4,x
(2xz| 1/2,1/2,1/2)

For 1' + set

(1) 1'
(1| 0,0,0)

(2) 2' 0,0,z
(2z| 0,0,0)

(3) 2' 0,y,0
(2y| 0,0,0)

(4) 2' x,0,0
(2x| 0,0,0)

(5) 3' x,x,x
(3xyz| 0,0,0)

(6) 3' x,x,x
(3xyz^-1| 0,0,0)

(7) 3' x,x,x
(3xyz| 0,0,0)

(8) 3' x,x,x
(3xyz^-1| 0,0,0)

(9) 3' x,x,x
(3xyz| 0,0,0)

(10) 3' x,x,x
(3xyz^-1| 0,0,0)

(11) 3' x,x,x
(3xyz| 0,0,0)

(12) 3' x,x,x
(3xyz^-1| 0,0,0)

(13) 2' (1/2,1/2,0) x,x,1/4
(2xy| 1/2,1/2,1/2)

(14) 2' x,x+1/2,1/4
(2xy| 1/2,1/2,1/2)

(15) 4' (0,0,1/2) 1/2,0,z
(4z^-1| 1/2,1/2,1/2)

(16) 4' (0,0,1/2) 0,1/2,z
(4z| 1/2,1/2,1/2)

(17) 4' (1/2,0,0) x,1/2,0
(4x^-1| 1/2,1/2,1/2)

(18) 2' (0,1/2,1/2) 1/4,y,y
(2yz| 1/2,1/2,1/2)

(19) 2' 1/4,y+1/2,y
(2yz| 1/2,1/2,1/2)

(20) 4' (1/2,0,0) x,0,1/2
(4x| 1/2,1/2,1/2)

(21) 4' (0,1/2,0) 1/2,y,0
(4y| 1/2,1/2,1/2)

(22) 2' (1/2,0,1/2) x,1/4,x
(2xz| 1/2,1/2,1/2)

(23) 4' (0,1/2,0) 0,y,1/2
(4y^-1| 1/2,1/2,1/2)

(24) 2' x,x+1/2,1/4,x
(2xz| 1/2,1/2,1/2)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 m 11'</td>
<td></td>
</tr>
</tbody>
</table>

(1) x,y,z  0,0,0
(2) x,y,z  0,0,0
(3) x,y,z  0,0,0
(4) x,y,z  0,0,0

(5) z,x,y  0,0,0
(6) z,x,y  0,0,0
(7) z,x,y  0,0,0
(8) z,x,y  0,0,0

(9) y,z,x  0,0,0
(10) y,z,x  0,0,0
(11) y,z,x  0,0,0
(12) y,z,x  0,0,0

(13) y+1/2,x+1/2,z+1/2 0,0,0
(14) y+1/2,x+1/2,z+1/2 0,0,0
(15) y+1/2,x+1/2,z+1/2 0,0,0
(16) y+1/2,x+1/2,z+1/2 0,0,0

(17) x+1/2,z+1/2,y+1/2 0,0,0
(18) x+1/2,z+1/2,y+1/2 0,0,0
(19) x+1/2,z+1/2,y+1/2 0,0,0
(20) x+1/2,z+1/2,y+1/2 0,0,0

(21) z+1/2,y+1/2,x+1/2 0,0,0
(22) z+1/2,y+1/2,x+1/2 0,0,0
(23) z+1/2,y+1/2,x+1/2 0,0,0
(24) z+1/2,y+1/2,x+1/2 0,0,0

12 l ..21' 1/4,y,y+1/2 0,0,0
(25) 3/4,y,y+1/2 0,0,0
(26) 3/4,y,y+1/2 0,0,0
(27) 1/4,y,y+1/2 0,0,0
(28) y+1/2,1/4,y 0,0,0
(29) y+1/2,1/4,y 0,0,0
(30) y+1/2,1/4,y 0,0,0
(31) y+1/2,1/4,y 0,0,0
(32) y+y+1/2,3/4,y 0,0,0
(33) y+y+1/2,3/4,y 0,0,0
(34) y+y+1/2,3/4,y 0,0,0
(35) y+y+1/2,3/4,y 0,0,0
Symmetry of Special Projections

Along [0,0,1] p4mm\(^{1'}\)

\(a^* = a\) \quad b^* = b\)

Origin at 0,1/2,z

Along [1,1,1] p3m1\(^{1'}\)

\(a^* = (2a - b - c)/3\) \quad b^* = (-a + 2b - c)/3\)

Origin at x,x,x

Along [1,1,0] p2mm\(^{1'}\)

\(a^* = (a + b)/2\) \quad b^* = c\)

Origin at x,x,1/4

P4\(_{2}\), 321'

4'32'

Cubic

208.3.1548 - 1 - 3461
Origin at 23

**Asymmetric unit**
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad \max (-x, x-1/2, -y, y-1/2) \leq z \leq \min (x, 1/2-x, y, 1/2-y) \]

**Vertices**
0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/4,1/4,1/4 1/4,1/4,-1/4

**Symmetry Operations**
(1) 1
(1 | 0,0,0)

(2) 2 0,0,z
(2 | z | 0,0,0)

(3) 2 0,y,0
(2 | y | 0,0,0)

(4) 2 x,0,0
(2 | z | 0,0,0)

(5) 3^+ x,x,x
(3_{xyz} | 0,0,0)

(6) 3^+ x,\bar{x},\bar{x}
(3_{xyz}^{-1} | 0,0,0)

(7) 3^+ x,\bar{x},\bar{x}
(3_{xyz}^{-1} | 0,0,0)

(8) 3^+ \bar{x},x,x
(3_{xyz}^{-1} | 0,0,0)

(9) 3^- x,x,x
(3_{xyz}^{-1} | 0,0,0)

(10) 3^- x,\bar{x},\bar{x}
(3_{xyz} | 0,0,0)

(11) 3^- \bar{x},x,x
(3_{xyz} | 0,0,0)

(12) 3^- \bar{x},\bar{x},\bar{x}
(3_{xyz} | 0,0,0)

**Continued**

208.3.1548 P4_{1}^{\prime}32'
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Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

**Positions**

Multiplicity,
Wyckoff letter,
Site Symmetry.

24 m 1

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) x,y,z [u,v,w]
(4) x,y,z [u,v,w]
(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]
(9) y,z,x [v,w,u]
(10) y,z,x [v,w,u]
(11) y,z,x [v,w,u]
(12) y,z,x [v,w,u]
(13) y+1/2,x+1/2,z+1/2 [v,u,w]
(14) y+1/2,x+1/2,z+1/2 [v,u,w]
(15) y+1/2,x+1/2,z+1/2 [v,u,w]
(16) y+1/2,x+1/2,z+1/2 [v,u,w]
(17) x+1/2,z+1/2,y+1/2 [u,w,v]
(18) x+1/2,z+1/2,y+1/2 [u,w,v]
(19) x+1/2,z+1/2,y+1/2 [u,w,v]
(20) x+1/2,z+1/2,y+1/2 [u,w,v]
(21) z+1/2,y+1/2,x+1/2 [w,v,u]
(22) z+1/2,y+1/2,x+1/2 [w,v,u]
(23) z+1/2,y+1/2,x+1/2 [w,v,u]
(24) z+1/2,y+1/2,x+1/2 [w,v,u]

208.3.1548 - 3 - 3463
Continued 208.3.1548 P4₁'2'32'

12 h 2.. \(x,0,0\) \([u,0,0]\) \(\bar{x},0,0\) \([\bar{u},0,0]\) \(0,x,0\) \([0,u,0]\) \(0,\bar{x},0\) \([0,\bar{u},0]\)
0,0,x \([0,0,u]\) 0,0,\(\bar{x}\) \([0,0,\bar{u}]\) 1/2,x+1/2,1/2 \([0,\bar{u},0]\) 1/2,\(\bar{x}\)+1/2,1/2 \([0,u,0]\)
\(x+1/2,1/2,1/2\) \([\bar{u},0,0]\) \(\bar{x}+1/2,1/2,1/2\) \([\bar{u},0,0]\) 1/2,1/2,\(x+1/2\) \([0,0,u]\) 1/2,1/2,\(x+1/2\) \([0,0,\bar{u}]\)

8 g .3. \(x,\bar{x},x\) \([u,u,u]\) \(\bar{x},\bar{x},x\) \([u,\bar{u},u]\)
\(x+1/2,\bar{x}+1/2,\bar{x}+1/2\) \([\bar{u},u,u]\) \(\bar{x}+1/2,\bar{x}+1/2,\bar{x}+1/2\) \([u,u,u]\)
\(x+1/2,\bar{x}+1/2,x+1/2\) \([\bar{u},u,u]\) \(\bar{x}+1/2,\bar{x}+1/2,x+1/2\) \([u,u,u]\)

6 f 2.2"2' 1/4,1/2,0 \([u,0,0]\) 3/4,1/2,0 \([u,0,0]\) 0,1/4,1/2 \([0,u,0]\)
0,3/4,1/2 \([0,\bar{u},0]\) 1/2,0,1/4 \([0,0,u]\) 1/2,0,3/4 \([0,0,\bar{u}]\)

6 e 2.2"2' 1/4,0,1/2 \([u,0,0]\) 3/4,0,1/2 \([u,0,0]\) 1/2,1/4,0 \([0,u,0]\)
1/2,3/4,0 \([0,\bar{u},0]\) 0,1/2,1/4 \([0,0,u]\) 0,1,2/3 \([0,0,\bar{u}]\)

6 d 222.. 0,1/2,1/2 \([0,0,0]\) 1/2,0,1/2 \([0,0,0]\) 1/2,1/2,0 \([0,0,0]\)
0,1/2,0 \([0,0,0]\) 1/2,0,0 \([0,0,0]\) 0,0,1/2 \([0,0,0]\)

4 c .32' 3/4,3/4,3/4 \([u,u,u]\) 1/4,1/4,3/4 \([\bar{u},\bar{u},u]\) 1/4,3/4,1/4 \([\bar{u},\bar{u},u]\) 3/4,1/4,1/4 \([u,\bar{u},\bar{u}]\)

4 b .32' 1/4,1/4,1/4 \([u,u,u]\) 3/4,3/4,1/4 \([\bar{u},\bar{u},u]\) 3/4,1/4,3/4 \([\bar{u},\bar{u},u]\) 1/4,3/4,3/4 \([u,\bar{u},\bar{u}]\)

2 a 23. 0,0,0 \([0,0,0]\) 1/2,1/2,1/2 \([0,0,0]\)

Symmetry of Special Projections

Along \([0,0,1]\) \(p4 \prime m \prime m\) \(a^* = a\) \(b^* = b\)
Origin at 0,1/2,z

Along \([1,1,1]\) \(p3 \prime m1\) \(a^* = (2a - b - c)/3\) \(b^* = (-a + 2b - c)/3\)
Origin at \(x,x,x\)

Along \([1,1,0]\) \(p2 \prime m \prime m\) \(a^* = c\) \(b^* = -(a + b)/2\)
Origin at \(x,x,1/4\)
**Origin** at 23

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad \max (-x, x-1/2, -y, y-1/2) \leq z \leq \min (x, 1/2-x, y, 1/2-y) \]

**Vertices**

- \(0,0,0\)
- \(1/2,0,0\)
- \(1/2,1/2,0\)
- \(0,1/2,0\)
- \(1/4,1/4,1/4\)
- \(1/4,1/4,-1/4\)

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \(1\)
   
2. \(2\) \(0,0,z\)
   
3. \(2\) \(y,0,0\)
   
4. \(2\) \(x,0,0\)
   
5. \(3^+\) \(x,x,x\)
   
6. \(3^+\) \(x,x,x\)
   
7. \(3^+\) \(x,x,x\)
   
8. \(3^+\) \(x,x,x\)

9. \(3^-\) \(x,x,x\)

10. \(3^-\) \(x,x,x\)

11. \(3^-\) \(x,x,x\)

12. \(3^-\) \(x,x,x\)
Symmetry of Special Projections

Along [0,0,1]  p4mm1'
\( a^* = a \quad b^* = b \)
Origin at 0,1/2,z

Along [1,1,1]  p3m11'
\( a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \)
Origin at x,x,x

Along [1,1,0]  p\_c\_2mm
\( a^* = (-a + b)/2 \quad b^* = c \)
Origin at x-1/4,x+1/4,3/4
209.1.1550 - 1 - 3469

**Origin** at 432

**Asymmetric unit**

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x, 1/2-x); \quad -y \leq z \leq y
\]

**Vertices**

<p>| | | | |</p>
<table>
<thead>
<tr>
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<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>1/4,1/4,1/4</td>
<td>1/4,1/4,-1/4</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

For \((0,0,0) + \text{set} \)

\[
\begin{align*}
(1) & \quad 1 \\
(1 & \ 0,0,0) \\
(2) & \quad 2 \ 0,0,z \\
(2_z & \ 0,0,0) \\
(3) & \quad 2 \ 0,y,0 \\
(2_y & \ 0,0,0) \\
(4) & \quad 2 \ x,0,0 \\
(2_x & \ 0,0,0) \\
(5) & \quad 3^+ \ x,x,x \\
(3_{xyz} & \ 0,0,0) \\
(6) & \quad 3^+ \ x,x,x \\
(3_{xyz}^{-1} & \ 0,0,0) \\
(7) & \quad 3^+ \ x,x,x \\
(3_{xyz}^{-1} & \ 0,0,0) \\
(8) & \quad 3^+ \ x,x,x \\
(3_{xyz}^{-1} & \ 0,0,0) \\
(9) & \quad 3^- \ x,x,x \\
(3_{xyz}^{-1} & \ 0,0,0) \\
(10) & \quad 3^- \ x,x,x \\
(3_{xyz} & \ 0,0,0) \\
(11) & \quad 3^- \ x,x,x \\
(3_{xyz} & \ 0,0,0) \\
(12) & \quad 3^- \ x,x,x \\
(3_{xyz} & \ 0,0,0)
\end{align*}
\]
Continued

(13) 2 x.x,0
      (2xy|0,0,0) (14) 2 x.x,0
      (2xy|0,0,0) (15) 4* 0,0,z
      (4z|0,0,0) (16) 4* 0,0,z
      (4z|0,0,0)

(17) 4* x,0,0
      (4x|0,0,0) (18) 2 0,y,y
      (2yz|0,0,0) (19) 2 0,y,y
      (2yz|0,0,0) (20) 4* x,0,0
      (4x|0,0,0)

(21) 4* y,0,0
      (4y|0,0,0) (22) 2 x,0,x
      (2xz|0,0,0) (23) 4* y,0,0
      (4y|0,0,0) (24) 2 x+1/2,0,x
      (2xz|0,0,0)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (2) 2 (0,0,1/2) 0,1/4,z
      (2z|0,1/2,1/2) (3) 2 (0,1/2,0) 0,y,1/4
      (2y|0,1/2,1/2) (4) 2 x,1/4,1/4
      (2xz|0,1/2,1/2)

(5) 3* (1/3,1/3,1/3)
      x-1/3,x-1/6,x (6) 3* x,x+1/2,
      x (7) 3* (-1/3,1/3,1/3)
      x+1/3,x-1/6,x
      (3xyz|0,1/2,1/2) (3xyz|0,1/2,1/2) (3xyz|0,1/2,1/2)

(9) 3* (1/3,1/3,1/3)
      x-1/6,x+1/6,x (10) 3* x+1/4,1/4,x
      (3xyz|0,1/2,1/2) (3xyz|0,1/2,1/2)

(13) 2 (1/4,1/4,0)
      x,x+1/4,1/4 (14) 2 (-1/4,1/4,0)
      x,x+1/4,1/4 (15) 4* (0,0,1/2) 1/4,1/4,z
      (2xy|0,1/2,1/2) (2y|0,1/2,1/2) (4z|0,1/2,1/2)

(17) 4* x,1/2,0
      (4x|0,1/2,1/2) (18) 2 (0,1/2,1/2) 0,y,y
      (2yz|0,1/2,1/2) (19) 2 0,y+1/2,y
      (2yz|0,1/2,1/2) (20) 4* x,0,1/2
      (4x|0,1/2,1/2)

(21) 4* (0,1/2,0)
      1/4,y,1/4 (22) 2 (1/4,0,1/4)
      x,1/4,1/4,x (23) 4* (0,1/2,0)
      -1/4,y,1/4
      (2yz|0,1/2,1/2) (4y|0,1/2,1/2)

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2) (2) 2 (0,0,1/2) 1/4,0,z
      (2z|1/2,0,1/2) (3) 2 1/4,y,1/4
      (2y|1/2,0,1/2) (4) 2 (1/2,0,0)
      x,0,1/4
      (2z|1/2,0,1/2)

(5) 3* (1/3,1/3,1/3)
      x+1/6,x+1/6,x (6) 3* x+1/2,
      x (7) 3* x+1/2,x
      x+1/3,x-1/6,x
      (3xyz|1/2,0,1/2) (3xyz|1/2,0,1/2) (3xyz|1/2,0,1/2)

(9) 3* (1/3,1/3,1/3)
      x-1/6,x+1/3,x (10) 3* x+1/2, 
      x (11) 3* x+1/2,
      x (12) 3* x-1/6,x-1/3,x
      (3xyz|1/2,0,1/2) (3xyz|1/2,0,1/2)

(13) 2 (1/4,1/4,0)
      x,x-1/4,1/4 (14) 2 (1/4,-1/4,0)
      x,x+1/4,1/4 (15) 4* (0,0,1/2) 1/4,-1/4,z
      (2xy|1/2,0,1/2) (2y|1/2,0,1/2) (4z|1/2,0,1/2)

(17) 4* (1/2,0,0)
      1/4,y,1/4 (18) 2 (0,1/4,1/4)
      x,-1/4,1/4 (19) 2 (0,-1/4,1/4)
      x,-1/4,1/4
      (2yz|1/2,0,1/2) (2yz|1/2,0,1/2)

(21) 4* y,0,0
      (4y|1/2,0,1/2) (22) 2 (1/2,0,1/2) x,0,x
      (2xz|1/2,0,1/2) (23) 4* y,0,1/2
      (4y|1/2,0,1/2) (24) 2 x+1/2,0,x
      (2xz|1/2,0,1/2)
Continued 209.1.1550 F432

For \((1/2,1/2,0) + \text{set}\)

(1) \(t\) \((1/2,1/2,0)\) 
(1) \(t\) \((1/2,1/2,0)\)
(2) \(2\) \((1/4,1/4,z)\) 
(2) \((1/2,1/2,0)\)
(3) \(2(0,1/2,0)\) \((1/4,y,0)\)
(3) \((2,1/2,0)\)
(4) \(2\) \((1/2,0,0)\) \((x,1/4,0)\)
(4) \((1/2,1/2,0)\)

(5) \(3^+\) \((1/3,1/3,1/3)\) 
(6) \(3^+\) \(\vec{x}+1/2,\vec{x}\)
(7) \(3^+\) \(\vec{x}+1/2,\vec{x}\)
(8) \(3^+\) \((1/3,1/3,-1/3)\)

(9) \(3^+\) \((1/3,1/3,1/3)\) 
(10) \(3^+\) \(x,\vec{x}+1/2,\vec{x}\)
(11) \(3^+\) \((1/3,1/3,-1/3)\)
(12) \(3^+\) \(x,\vec{x}+1/2,\vec{x}\)

(13) \(2\) \((1/2,1/2,0)\) \((x,x,0)\)
(14) \(2\) \((x,x,1/2,0)\)
(15) \(4^+\) \((1/2,0,z)\)
(16) \(4^+\) \((0,1/2,z)\)

(17) \(4^+\) \((1/2,0,0)\) \((x,1/4,-1/4)\)
(18) \(2\) \((0,1/4,1/4)\)
(19) \(2\) \((0,1/4,-1/4)\)
(20) \(4^+\) \((1/2,0,0)\) \((x,1/4,1/4)\)

(21) \(4^+\) \((0,1/2,0)\) \((1/4,y,-1/4)\)
(22) \(2\) \((1/4,0,1/4)\)
(23) \(4^+\) \((0,1/2,0)\) \((1/4,y,1/4)\)
(24) \(2\) \((1/4,0,-1/4)\)

Generators selected \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).\)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

96 \(j\) 1

(1) \(x,y,z\) \([u,v,w]\)
(2) \(\vec{x},\vec{y},\vec{z}\) \([\vec{u},\vec{v},\vec{w}]\)
(3) \(\vec{x},y,\vec{z}\) \([\vec{u},v,w]\)
(4) \(x,y,\vec{z}\) \([u,v,\vec{w}]\)

(5) \(z,x,y\) \([w,u,v]\)
(6) \(z,\vec{x},\vec{y}\) \([w,\vec{u},\vec{v}]\)
(7) \(\vec{z},\vec{x},y\) \([\vec{w},u,v]\)
(8) \(\vec{z},x,\vec{y}\) \([\vec{w},u,\vec{v}]\)

(9) \(y,z,x\) \([v,w,u]\)
(10) \(\vec{y},\vec{z},\vec{x}\) \([\vec{v},\vec{w},\vec{u}]\)
(11) \(y,z,\vec{x}\) \([v,\vec{w},u]\)
(12) \(\vec{y},z,x\) \([\vec{v},w,u]\)

(13) \(x,y,\vec{z}\) \([v,u,\vec{w}]\)
(14) \(\vec{x},y,\vec{z}\) \([\vec{v},u,\vec{w}]\)
(15) \(y,\vec{x},z\) \([v,\vec{u},w]\)
(16) \(\vec{y},x,z\) \([\vec{v},u,\vec{w}]\)

(17) \(x,z,y\) \([u,w,v]\)
(18) \(\vec{x},\vec{z},y\) \([\vec{u},w,\vec{v}]\)
(19) \(x,\vec{z},y\) \([u,\vec{w},v]\)
(20) \(x,z,\vec{y}\) \([u,v,\vec{w}]\)

(21) \(z,y,\vec{x}\) \([w,v,u]\)
(22) \(z,\vec{y},x\) \([w,\vec{v},u]\)
(23) \(\vec{z},y,\vec{x}\) \([\vec{w},v,u]\)
(24) \(\vec{z},\vec{y},\vec{x}\) \([\vec{w},\vec{v},\vec{u}]\)

48 \(i\) 2

48 \(h\) 2

Axes, \(x,1/4,1/4 [u,0,0]\) \(x,3/4,1/4 [u,0,0]\) \(1/4,x,1/4 [0,u,0]\) \(1/4,x,3/4 [0,u,0]\)

\(3/4,1/4,x [0,0,u]\) \(1/4,x,3/4 [0,u,0]\)

\(1/4,3/4,x [u,0,0]\) \(1/4,1/4,x [0,0,u]\)
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<th>g</th>
<th>0.y.y [0,v,v]</th>
<th>0.v.y [0,v,v]</th>
<th>0.v.y [0,v,v]</th>
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<td>y.y.0 [v,0,0]</td>
<td>y.y.0 [v,0,0]</td>
<td>y.y.0 [v,0,0]</td>
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<td>32</td>
<td>f</td>
<td>x.x.x [u,u,u]</td>
<td>x.x.x [u,u,u]</td>
<td>x.x.x [u,u,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x.x.0 [u,u,u]</td>
<td>x.x.0 [u,u,u]</td>
<td>x.x.0 [u,u,u]</td>
</tr>
<tr>
<td>24</td>
<td>e</td>
<td>x.0,0 [u,0,0]</td>
<td>0.x.0 [u,0,0]</td>
<td>0.0.x [u,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.x.0 [u,0,0]</td>
<td>0.x.0 [u,0,0]</td>
<td>0.x.0 [u,0,0]</td>
</tr>
<tr>
<td>24</td>
<td>d</td>
<td>0.1/4,1/4 [0,0,0]</td>
<td>0.3/4,1/4 [0,0,0]</td>
<td>1/4,0,1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/4,0,1/4 [0,0,0]</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>8</td>
<td>c</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>b</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4</td>
<td>a</td>
<td>0.0,0 [0,0,0]</td>
<td>0.0,0 [0,0,0]</td>
<td>0.0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]** p4m'm'
  - \( a^* = a/2 \quad b^* = b/2 \)
  - Origin at 0,0,z

- **Along [1,1,1]** p3m'1
  - \( a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6 \)
  - Origin at x,x,x

- **Along [1,1,0]** c2m'm'
  - \( a^* = (-a + b)/2 \quad b^* = c \)
  - Origin at x,x,0
Origin at 4321'

Asymmetric unit
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad -y \leq z \leq y \]

Vertices
\[ 0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4 \]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
& \quad (1 | 0,0,0) \\
(2) & \quad \bar{z} \quad (2_z | 0,0,0) \\
(3) & \quad y \quad (2_y | 0,0,0) \\
(4) & \quad x \quad (2_x | 0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz} | 0,0,0) \\
(6) & \quad 3^+ \quad \bar{x},\bar{x},\bar{x} \\
& \quad (3_{xyz}^{-1} | 0,0,0) \\
(7) & \quad \bar{y} \quad (3_y | 0,0,0) \\
(8) & \quad \bar{x} \quad (3_x | 0,0,0) \\
(9) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz}^{-1} | 0,0,0) \\
(10) & \quad 3^- \quad \bar{x},\bar{x},\bar{x} \\
& \quad (3_{xyz} | 0,0,0) \\
(11) & \quad \bar{x} \quad (3_x | 0,0,0) \\
(12) & \quad \bar{y} \quad (3_y | 0,0,0)
\end{align*}
\]
Continued

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (1) t (0,1/2,1/2)  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4
(1) 0,1/2,1/2)  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4  (2) 0,1/2,1/2  (2) 2 (0,0,1/2) 0,1/4,z  (3) 2 (0,1/2,0) 0,y,1/4  (4) 2 x,1/4,1/4
Continued

(13) \(2' \cdot (1/4,1/4,0)\) \(x,x+1/4,1/4\)  
(14) \(2' \cdot (-1/4,1/4,0)\) \(x\bar{x}+1/4,1/4\)  
(15) \(4' \cdot (0,0,1/2)\) \(1/4,1/4,z\)  
(16) \(4' \cdot (0,0,1/2)\) \(-1/4,1/4,z\)

(17) \(4' \cdot (x,1/2,0)\)  
(18) \(2' \cdot (0,1/2,1/2)\) \(0,y,y\)  
(19) \(2' \cdot y,+1/2,\bar{y}\) \(2y\) \(0,1/2,1/2)\) \(0,1/2,1/2)\)

(20) \(4' \cdot x,0,1/2)\)

(21) \(4' \cdot (0,1/2,0)\) \(1/4,y,1/4\)  
(22) \(2' \cdot (1/4,0,1/4)\) \(x-1/4,1/4,x\)  
(23) \(4' \cdot (0,1/2,0)\) \(-1/4,y,1/4\)  
(24) \(2' \cdot (-1/4,0,1/4)\) \(x+1/4,1/4,x\)

(209.2.1551 - 4 - 3476)

Continued

(1) \(t' \cdot (1/2,0,1/2)\)  
(2) \(2' \cdot (0,0,1/2)\) \(1/4,0,z\)  
(3) \(2' \cdot 1/4,y,1/4\)  
(4) \(2' \cdot (1/2,0,1/2)\)

(5) \(3' \cdot (1/3,3/1,3)\) \(x+1/6,x-1/6,x\)  
(6) \(3' \cdot (1/3,-1/3,1/3)\) \(x+1/6,x+1/6,x\)

(7) \(3' \cdot x+1/2,x-1/2,x\)

For \((1/2,0,1/2)\) + set

(13) \(2' \cdot (1/4,1/4,0)\) \(x,x-1/4,1/4\)  
(14) \(2' \cdot (1/4,-1/4,0)\) \(x\bar{x}+1/4,1/4\)  
(15) \(4' \cdot (0,0,1/2)\) \(1/4,-1/4,z\)  
(16) \(4' \cdot (0,0,1/2)\) \(1/4,1/4,z\)

(17) \(4' \cdot (1/2,0,0)\) \(x,1/4,1/4\)  
(18) \(2' \cdot (0,1/4,1/4)\) \(1/4,y,1/4\)  
(19) \(2' \cdot (0,-1/4,1/4)\) \(1/4,y+1/4,y\)

(20) \(4' \cdot (1/2,0,0)\) \(x,-1/4,1/4\)  
(4' \cdot (1/2,0,1/2)\)

(21) \(4' \cdot (1/2,y,0)\) \(4' \cdot y,1/2,0\)  
(22) \(2' \cdot (1/2,0,1/2)\) \(x,0,x\)  
(23) \(4' \cdot 0,y,1/2\)  
(24) \(2' \cdot \bar{x}+1/2,0,x\)

For \((1/2,1/2,0)\) + set

(1) \(t' \cdot (1/2,1/2,0)\)  
(2) \(2' \cdot 1/4,1/4,z\)  
(3) \(2' \cdot (0,1/2,0)\) \(1/4,y,0\)  
(4) \(2' \cdot (1/2,0,0)\) \(x,1/4,0\)

(5) \(3' \cdot (1/3,1/3,1/3)\) \(x+1/6,x+1/3,x\)  
(6) \(3' \cdot x+1/2,x,\bar{x}\)

For \((1/2,1/2,0)\) + set

(13) \(2' \cdot (1/2,1/2,0)\) \(x,x,0\)  
(14) \(2' \cdot x,\bar{x}+1/2,0\)  
(15) \(4' \cdot 1/2,0,z\)  
(16) \(4' \cdot 0,1/2,z\)

(17) \(4' \cdot (1/2,0,0)\) \(x,1/4,-1/4\)  
(18) \(2' \cdot (0,1/4,1/4)\) \(1/4,y+1/4,y\)  
(19) \(2' \cdot (0,1/4,-1/4)\) \(1/4,y+1/4,y\)

(20) \(4' \cdot (1/2,0,0)\) \(x,1/4,1/4\)  
(4' \cdot (1/2,1/2,0)\)

(21) \(4' \cdot (0,1/2,0)\) \(1/4,y,-1/4\)  
(22) \(2' \cdot (1/4,0,1/4)\) \(x+1/4,1/4,x\)  
(23) \(4' \cdot (0,1/2,0)\) \(1/4,y,1/4\)  
(24) \(2' \cdot (1/4,0,-1/4)\) \(x+1/4,1/4,x\)

Generators selected \(1); t(1,0,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); 1'.
<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity, Wyckoff letter, Site Symmetry.</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + (0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + (0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>96 j 11'</td>
<td>(1) x,y,z [0,0,0]  (2) x, y,z [0,0,0]  (3) x,y, z [0,0,0]  (4) x, y, z [0,0,0]  (5) z,x,y [0,0,0]  (6) z, x,y [0,0,0]  (7) z, x, y [0,0,0]  (8) z, x, y [0,0,0]  (9) y,z,x [0,0,0]  (10) y, z,x [0,0,0]  (11) y, z, x [0,0,0]  (12) y, z, x [0,0,0]  (13) y,x, z [0,0,0]  (14) y, x, z [0,0,0]  (15) y, x, z [0,0,0]  (16) y, x, z [0,0,0]  (17) x,z, y [0,0,0]  (18) x, z, y [0,0,0]  (19) x, z, y [0,0,0]  (20) x, z, y [0,0,0]  (21) z,y,x [0,0,0]  (22) z, y,x [0,0,0]  (23) z, y,x [0,0,0]  (24) z, y,x [0,0,0]</td>
</tr>
<tr>
<td>48 i 2..1'</td>
<td>x,1/4,1/4 [0,0,0]  x,3/4,1/4 [0,0,0]  1/4,x,1/4 [0,0,0]  1/4,x,3/4 [0,0,0]  1/4,3/4,x [0,0,0]  1/4,3/4,1/4 [0,0,0]  1/4,1/4,x [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,1/4 [0,0,0]  1/4,3/4,1/4 [0,0,0]  1/4,3/4,3/4 [0,0,0]  1/4,3/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>48 h ..21'</td>
<td>1/2,y,y [0,0,0]  1/2, y,y [0,0,0]  1/2,y, y [0,0,0]  1/2, y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]  1/2,y, y [0,0,0]</td>
</tr>
<tr>
<td>48 g ..21'</td>
<td>0,y,y [0,0,0]  0, y,y [0,0,0]  0,y, y [0,0,0]  0, y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]  0,y, y [0,0,0]</td>
</tr>
<tr>
<td>32 f .3.1'</td>
<td>x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]  x,x,x [0,0,0]</td>
</tr>
<tr>
<td>24 e 4..1'</td>
<td>x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]  x,0,0 [0,0,0]</td>
</tr>
<tr>
<td>24 d 2.221'</td>
<td>0,1/4,1/4 [0,0,0]  0,3/4,1/4 [0,0,0]  1/4,0,1/4 [0,0,0]  1/4,0,1/4 [0,0,0]  1/4,3/4,0 [0,0,0]  1/4,3/4,1/4 [0,0,0]  3/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>8 c 23.1'</td>
<td>1/4,1/4,1/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>4 b 4321'</td>
<td>1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>4 a 4321'</td>
<td>0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

Along [0,0,1] p4mm1'
\[a^* = a/2 \quad b^* = b/2\]
Origin at 0,0,z

Along [1,1,1] p3m11'
\[a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6\]
Origin at x,x,x

Along [1,1,0] c2mm1'
\[a^* = (-a + b)/2 \quad b^* = c\]
Origin at x,x,0
Origin at 4'32'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x, 1/2-x); \quad -y \leq z \leq y \]

Vertices

\( 0,0,0 \) \hspace{0.5cm} 1/2,0,0 \hspace{0.5cm} 1/4,1/4,1/4 \hspace{0.5cm} 1/4,1/4,-1/4

Symmetry Operations

For \((0,0,0) + \text{set}\)

\begin{align*}
(1) & \quad 1 \\
& \quad (1 | 0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2_z | 0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz} | 0,0,0) \\
(6) & \quad 3^{-} \quad x,x,x \\
& \quad (3_{xyz}^{-1} | 0,0,0) \\
(9) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz} | 0,0,0) \\
(10) & \quad 3^{-} \quad x,x,x \\
& \quad (3_{xyz}^{-1} | 0,0,0) \\
(11) & \quad 2 \quad x,0,0 \\
& \quad (2_z | 0,0,0) \\
(12) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz} | 0,0,0)
\end{align*}
For $(1/2,1/2,0) + \text{set}$

$(1) \ t(1/2,1/2,0) \quad (2) \ 2 \ 1/4,1/4,z \quad (3) \ 2 \ (0,1/2,0) \ 1/4,y,0 \quad (4) \ 2 \ (1/2,0,0) \ x,1/4,0$

$(1) \ |1/2,1/2,0) \quad (2) \ z,1/2,1/2,0) \quad (3) \ y,1/2,1/2,0) \quad (4) \ x,1/2,1/2,0) \quad (5) \ z,x,y [w,u,v] \quad (6) \ z,x,y [v,u,w] \quad (7) \ z,x,y [v,w,u] \quad (8) \ z,x,y [u,v,w] \quad (9) \ z,x,y [u,w,v] \quad (10) \ z,x,y [v,w,u] \quad (11) \ z,x,y [v,u,w] \quad (12) \ z,x,y [v,u,w] \quad (13) \ z,x,y [u,w,v] \quad (14) \ z,x,y [v,w,u] \quad (15) \ z,x,y [w,u,v] \quad (16) \ z,x,y [w,v,u]$

$Generators selected \quad (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,0,1/2); t(1/2,1/2,0); (2); (3); (5); (13).$

| Positions |
| Coordinates |
| Multiplicity, Wyckoff letter, Site Symmetry. |
| 96 j 1 |

$(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +$
| 48 | g   | 0.2' | 0,y,y [u,v,v] | 0,y,y [u,v,v] | 0,y,y [u,v,v] |
|    |     |      | y,0,y [v,u,v] | y,0,y [v,u,v] | y,0,y [v,u,v] |
|    |     |      | y,y,0 [v,v,u] | y,y,0 [v,v,u] | y,y,0 [v,v,u] |
| 32 | f   | 0.3' | x,x,x [u,u,u] | x,x,x [u,u,u] | x,x,x [u,u,u] |
|    |     |      | x,x,x [u,u,u] | x,x,x [u,u,u] | x,x,x [u,u,u] |
| 24 | e   | 4.  | x,0,0 [u,0,0] | x,0,0 [u,0,0] | 0,x,0 [0,u,0] |
|    |     |      | 0,x,0 [0,u,0] | 0,x,0 [0,u,0] | 0,0,x [0,0,u] |
| 24 | d   | 2.2' | 0,1/4,1/4 [u,0,0] | 0,3/4,1/4 [u,0,0] | 1/4,0,1/4 [0,u,0] |
|    |     |      | 1/4,0,3/4 [0,u,0] | 1/4,1/4,0 [0,u,0] | 3/4,1/4,0 [0,0,u] |
| 8  | c   | 23. | 1/4,1/4,1/4 [0,0,0] | 1/4,1/4,3/4 [0,0,0] | 1/4,1/4,3/4 [0,0,0] |
| 4  | b   | 4'32' | 1/2,1/2,1/2 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |
| 4  | a   | 4'32' | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm  
\[ a^* = a/2 \hspace{1cm} b^* = b/2 \]
Origin at 0,0,z

Along [1,1,1] p3m1  
\[ a^* = (2a - b - c)/6 \hspace{1cm} b^* = (-a + 2b - c)/6 \]
Origin at x,x,x

Along [1,1,0] c2'mm'  
\[ a^* = -a/2 \hspace{1cm} b^* = -(-a + b)/2 \]
Origin at x,x,0
Origin at 23

Asymmetric unit
0 ≤ x ≤ 1/2; -1/8 ≤ y ≤ 1/8; -1/8 ≤ z ≤ 1/8; y ≤ min (x,1/2-x); -y ≤ z ≤ min (x,1/2-x)

Vertices
0,0,0 1/8,1/8,1/8 1/8,1/8,-1/8 1/8,-1/8,1/8 1/2,0,0 3/8,1/8,1/8 3/8,1/8,-1/8 3/8,-1/8,1/8

Symmetry Operations
For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 (0,0,1/2) 0,1/4,z
2z|0,1/2,1/2

(3) 2 (0,1/2,0) 1/4,y,0
2y|1/2,1/2,0

(4) 2 (1/2,0,0) x,0,1/4
2x|1/2,0,1/2

(5) 3+(x,x,x)

(6) 3+(1/3,-1/3,1/3)
3xz\|1/2,0,1/2

(7) 3+(1/3,1/3,-1/3)
3yz\|1/2,0,1/2

(8) 3+(1/3,1/3,-1/3)
3xyz\|1/2,1/2,0

(9) 3+(x,x,x)

(10) 3+(1/2,x,x)
3xy|0,1/2,1/2

(11) 3+(1/2,x,1/2)
3xy|0,1/2,1/2

(12) 3+(1/2,x,1/2)
3xy|0,1/2,1/2

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(13) 2 (1/2,1/2,0) x,x-1/4,3/8 \\
(2xy) | 3/4,1/4,3/4
(14) 2 x,x+1/4,1/8 \\
(2xy) | 1/4,1/4,1/4
(15) 4 (0,0,3/4) 1/2,1/4,z \\
(4z) | 1/4,3/4,3/4
(16) 4 (0,0,1/4) 0,3/4,z \\
(4z) | 3/4,3/4,1/4

(17) 4' (3/4,0,0) x,1/2,1/4 \\
(4x) | 3/4,1/4,3/4
(18) 2 (0,1/2,1/2) 3/8,y+1/4,y \\
(2yz) | 3/4,3/4,1/4
(19) 2 1/8,y+1/4, y \\
(2yz) | 1/4,1/4,1/4
(20) 4 (1/4,0,0) x,0,3/4 \\
(4x) | 1/4,3/4,3/4

(21) 4' (0,1/4,0) 3/4,y,0 \\
(4y) | 3/4,1/4,3/4
(22) 2 (1/2,0,1/2) x-1/4,3/8,x \\
(2xz) | 1/4,1/4,3/4
(23) 4' (0,3/4,0) 1/4,y,1/2 \\
(4y) | 3/4,3/4,1/4
(24) 2 x+1/4,1/8,x \\
(2xz) | 1/4,1/4,1/4

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) \\
(1) 0,1/2,1/2
(2) 2 0,0,z \\
(2z) | 0,0,0
(3) 2 1/4,y,1/4 \\
(2yz) | 1/2,0,1/2
(4) 2 (1/2,0,0) x,1/4,0 \\
(2z) | 1/2,1/2,0

(5) 3' (1/3,1/3,1/3) x-1/6,x+1/6,x \\
(3xyz) | 0,1/2,1/2
(6) 3' x+1/2,x,x \\
(3xyz) | 1/2,1/2,0
(7) 3' x,x,x \\
(3xyz) | 0,0,0
(8) 3' x+1/2,x+1/2,x \\
(3xyz) | 1/2,0,1/2

(9) 3' (1/3,1/3,1/3) x-1/6,x+1/6,x \\
(3xyz) | 0,1/2,1/2
(10) 3' x+1/2,x,x \\
(3xyz) | 1/2,0,1/2
(11) 3' x+1/2,x,x,x \\
(3xyz) | 0,0,0
(12) 3' x,x,x+1/2,x \\
(3xyz) | 1/2,1/2,0

(13) 2 (3/4,3,4,0) x,x,1/8 \\
(2xz) | 3/4,3,4,1/4
(14) 2 (-1/4,1,4,0) x,x+1/2,3/8 \\
(2yz) | 1/4,3,4,3/4
(15) 4' (0,0,1/4) 1/4,0,z \\
(4z) | 1/4,1/4,1/4
(16) 4' (0,0,3/4) 1/4,1/2,z \\
(4z) | 3/4,1/4,3/4

(17) 4' (3/4,0,0) x,1/2,-1/4 \\
(4x) | 3/4,3,4,1/4
(18) 2 (0,1/2,1/2) 3/8,y-1/4,y \\
(2yz) | 3/4,1/4,3/4
(19) 2 1/8,y+3/4, y \\
(2yz) | 1/4,3,4,3/4
(20) 4' (1/4,0,0) x,0,1/4 \\
(4x) | 1/4,1,4,1/4

(21) 4' (0,3/4,0) 1/2,y,-1/4 \\
(4y) | 3/4,3,4,1/4
(22) 2 (1/4,0,1/4) x,1/8,x \\
(2xz) | 1/4,1/4,1/4
(23) 4' (0,1/4,0) 0,y,3/4 \\
(4y) | 3/4,1/4,3/4
(24) 2 (-1/4,0,1/4) x+1/2,3/8,x \\
(2xz) | 1/4,3,4,3/4

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2) \\
(1) 1/2,0,1/2
(2) 2 1/4,1/4,z \\
(2z) | 1/2,1/2,0
(3) 2 0,1/2,0) 0,y,1/4 \\
(2yz) | 0,1/2,1/2
(4) 2 x,0,0 \\
(2z) | 0,0,0

(5) 3' (1/3,1/3,1/3) x+1/6,x-1/6,x \\
(3xyz) | 1/2,0,1/2
(6) 3' x,x,x \\
(3xyz) | 0,0,0
(7) 3' x+x+1/2,x,x \\
(3xyz) | 1/2,1/2,0
(8) 3' x,x+1/2,x \\
(3xyz) | 0,0,0

(9) 3' (1/3,1/3,1/3) x+1/6,x-1/6,x \\
(3xyz) | 1/2,0,1/2
(10) 3' (-1/3,1/3,1/3) x+1/6,x+1/6,x \\
(3xyz) | 1/2,1/2,0
(11) 3' x,x,x \\
(3xyz) | 0,0,0
(12) 3' x,x+1/2,x \\
(3xyz) | 1/2,1/2,0

(13) 2 (1/4,1,4,0) x,x,1/8 \\
(2xz) | 1/4,1,4,1/4
(14) 2 (1/4,-1/4,0) x,x+1/2,3/8 \\
(2yz) | 3/4,1/4,3/4
(15) 4 (0,0,1/4) 3/4,0,z \\
(4z) | 3/4,3/4,1/4
(16) 4 (0,0,3/4) -1/4,1/2,z \\
(4z) | 1/4,3,4,3/4

(17) 4' (1/4,0,0) x,1/4,0 \\
(4x) | 1/4,1,4,1/4
(18) 2 (0,3/4,3/4) 1/8,y,y \\
(2yz) | 1/4,3,4,3/4
(19) 2 0,-1/4,1/4) 3/8,y+1/2, y \\
(2yz) | 3/4,1/4,3/4
(20) 4' (3/4,0,0) x,1/4,1/2 \\
(4x) | 3/4,3,4,1/4

(21) 4' (0,1/4,0) 1/4,y,0 \\
(4y) | 1/4,1,4,1/4
(22) 2 (1/2,0,1/2) x+1/4,3/8,x \\
(2xz) | 3/4,3,4,1/4
(23) 4' (0,3/4,0) -1/4,y,1/2 \\
(4y) | 1/4,3,4,3/4
(24) 2 x+3/4,1/8,x \\
(2xz) | 1/4,1/4,3/4

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Continued

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  (2) 2 (0,0,1/2) 1/4,0,z  (3) 2 0,y,0  (4) 2 x,1/4,1/4
   (1|1/2,1/2,0)  (2z|1/2,0,1/2)  (2y|0,0,0)  (2x|0,1/2,1/2)

(5) 3* (1/3,1/3,1/3)  (6) 3* x,x+1/2,x  (7) 3* x+1/2,x-1/2,x  (8) 3* x,x,x
   x+1/6,x+1/3,x  (3xz|1/2,1/2,0)  (3xz⁻¹|0,1/2,1/2)  (3xz⁻¹|1/2,0,1/2)  (3xz⁻¹|0,0,0)

(9) 3* (1/3,1/3,1/3)  (10) 3* x,x,x  (11) 3* x+1/2,x+1/2,x  (12) 3* (1/3,-1/3,1/3)
   x+1/3,x+1/6,x  (3yz⁻¹|1/2,1/2,0)  (3yz|0,1,2,1/2)  (3yz|1/2,0,1/2)

(13) 2 (1/2,1/2,0)  (14) 2 x,x+3/4,1/8  (15) 4* (0,0,3/4) 1/2,-1/4,z  (16) 4* (0,0,1/4) 0,1/4,z
     x,x+1/4,3/8  (2xz|1/4,3/4,3/4)  (2xz|3/4,3/4,1/4)  (4z|1/4,1/4,1/4)

(17) 4* (1/4,0,0)  (18) 2 (0,1/4,1/4) 1/8,y,y  (19) 2 (0,1/4,-1/4) 3/8,y+1/2,y  (20) 4* (3/4,0,0) x,-1/4,1/2
     x,3/4,0  (4z⁻¹|1/4,3/4,3/4)  (2yz|1/4,1/4,1/4)  (4x|3/4,1/4,3/4)

(21) 4* (0,3/4,0)  (22) 2 (3/4,0,3/4) x,1/8,x  (23) 4* (0,1/4,0) 0,y,1/4  (24) 2 (1/4,0,-1/4)
     1/2,y,1/4  (4z⁻¹|1/4,1/4,1/4)  (2xz|3/4,3/4,1/4)

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Coordinate</th>
<th>(0,0,0) +</th>
<th>(0,1/2,1/2) +</th>
<th>(1/2,0,1/2) +</th>
<th>(1/2,1/2,0) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,y,z [u,v,w]</td>
<td>x,y+1/2,z+1/2 [u,v,w]</td>
<td>x+1/2,y+1/2,z [u,v,w]</td>
<td>x+1/2,y,z+1/2 [u,v,w]</td>
<td>x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>z,x,y [w,u,v]</td>
<td>z+1/2,x,y+1/2 [w,u,v]</td>
<td>z+1/2,x+1/2,y [w,u,v]</td>
<td>z+1/2,x+1/2,y [w,u,v]</td>
<td>z+1/2,x+1/2,y [w,u,v]</td>
</tr>
<tr>
<td>y,z,x [v,w,u]</td>
<td>y+1/2,z+1/2,x [v,w,u]</td>
<td>y+1/2,z+1/2,x [v,w,u]</td>
<td>y+1/2,z+1/2,x [v,w,u]</td>
<td>y+1/2,z+1/2,x [v,w,u]</td>
</tr>
<tr>
<td>y,z+1/2,x+1/4,3/4 [v,u,w]</td>
<td>y+1/2,x+1/4,3/4 [v,u,w]</td>
<td>y+1/2,x+1/4,3/4 [v,u,w]</td>
<td>y+1/2,x+1/4,3/4 [v,u,w]</td>
<td>y+1/2,x+1/4,3/4 [v,u,w]</td>
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<td>1/8,y,y+1/4,0 [v,v]</td>
<td>7/8,y+1/2,y+3/4,0 [v,v]</td>
<td>7/8,y+1/2,y+3/4,0 [v,v]</td>
<td>7/8,y+1/2,y+3/4,0 [v,v]</td>
<td>7/8,y+1/2,y+3/4,0 [v,v]</td>
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<tr>
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<td>1/8,y+1/4,1/8 [v,v,0]</td>
<td>1/8,y+1/4,1/8 [v,v,0]</td>
<td>1/8,y+1/4,1/8 [v,v,0]</td>
</tr>
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<td>1/4,0,0 [u,0,0]</td>
<td>1/4,0,0 [u,0,0]</td>
<td>1/4,0,0 [u,0,0]</td>
<td>1/4,0,0 [u,0,0]</td>
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<tr>
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<td>1/4,0,0 [0,u,0]</td>
<td>1/4,0,0 [0,u,0]</td>
<td>1/4,0,0 [0,u,0]</td>
<td>1/4,0,0 [0,u,0]</td>
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<td>1/4,0,0 [0,0,0]</td>
<td>1/4,0,0 [0,0,0]</td>
<td>1/4,0,0 [0,0,0]</td>
<td>1/4,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

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32 e .3. x,x,x [u,u,u] \[ \bar{x}, \bar{x}+1/2, x+1/2 [u,u,u] \]
\[ \bar{x}+1/2, x+1/2, x [u,u,u] \] \[ x+1/2, \bar{x}, x+1/2 [u,u,u] \]
\[ x+3/4, x+1/4, x+3/4 [u,u,\bar{u}] \] \[ \bar{x}+1/4, \bar{x}+1/4, x+1/4 [u,u,u] \]
\[ x+1/4, x+3/4, x+3/4 [u,u,u] \] \[ \bar{x}+3/4, x+3/4, x+1/4 [u,u,u] \]

16 d .32 5/8,5/8,5/8 [0,0,0] \[ 3/8,7/8,1/8 [0,0,0] \] \[ 7/8,1/8,3/8 [0,0,0] \] \[ 1/8,3/8,7/8 [0,0,0] \]

16 c .32 1/8,1/8,1/8 [0,0,0] \[ 7/8,3/8,5/8 [0,0,0] \] \[ 3/8,5/8,7/8 [0,0,0] \] \[ 5/8,7/8,3/8 [0,0,0] \]

8 b 23. 1/2,1/2,1/2 [0,0,0] \[ 1/4,3/4,1/4 [0,0,0] \]

8 a 23. 0,0,0 [0,0,0] \[ 3/4,1/4,3/4 [0,0,0] \]

**Symmetry of Special Projections**

Along [0,0,1] p4m' m'
\[ a^* = a/2 \quad b^* = b/2 \]
Origin at 1/4,0,z

Along [1,1,1] p3m'1
\[ a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6 \]
Origin at x,x,x

Along [1,1,0] c2m' m'
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,1/8
Origin at 231°

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad -1/8 \leq y \leq 1/8; \quad -1/8 \leq z \leq 1/8; \quad y \leq \min(x,1/2-x); \quad -y \leq z \leq \min(x,1/2-x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/8,1/8,1/8 & \quad 1/8,1/8,-1/8 & \quad 1/8,-1/8,1/8 & \quad 1/8,-1/8,1/8 \\
1/2,0,0 & \quad 3/8,1/8,1/8 & \quad 3/8,1/8,-1/8 & \quad 3/8,-1/8,1/8 & \quad 3/8,-1/8,1/8
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(1 \mid 0,0,0) & \quad (2) \quad 2 \ (0,0,1/2) \quad 0,1/4,z \\
(2z \mid 0,1/2,1/2) & \quad (3) \quad 2 \ (0,1/2,0) \quad 1/4,y,0 \\
(2y \mid 1/2,1/2,0) & \quad (4) \quad 2 \ (1/2,0,0) \quad x,0,1/4 \\
(2z \mid 1/2,0,1/2) & \quad (5) \quad 3^+ \ x,x,x \\
(6) \quad 3^+ \ (1/3,-1/3,1/3) \quad x+1/6,x+1/6,x & \quad (7) \quad 3^+ \ (-1/3,1/3,1/3) \quad x+1/3,x+1/6,x \\
(3_{xyz} \mid 1/2,0,1/2) & \quad (3_{xyz}^{-1} \mid 0,1/2,1/2) & \quad (3_{xyz}^{-1} \mid 1/2,1/2,0) \\
(8) \quad 3^+ \ (1/3,1/3,-1/3) \quad x+1/6,x+1/3,x & \quad (9) \quad 3^+ \ x,x,x \\
(3_{xyz}^{-1} \mid 0,0,0) & \quad (10) \quad 3^- \ x,x+1/2,x & \quad (11) \quad 3^- \ x+1/2,x,x \\
(3_{xyz} \mid 1/2,1/2,0) & \quad (3_{xyz} \mid 1/2,0,1/2) & \quad (3_{xyz} \mid 0,1/2,1/2) & \quad (3_{xyz} \mid 1/2,1/2,0) \\
(12) & \quad 3^- \ x-1/2,x+1/2,x
\end{align*}
\]
<table>
<thead>
<tr>
<th>(13)</th>
<th>2 (1/2, 1/2, 0)</th>
<th>x, x−1/4, 3/8 (2xy) 3/4, 1/4, 3/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>(14)</td>
<td>2 x, x+1/4, 1/8 (2xy) 1/4, 1/4, 1/4</td>
<td></td>
</tr>
<tr>
<td>(15)</td>
<td>4 (0, 0, 3/4) 1/2, 1/4, z (4z) 1/4, 3/4, 3/4</td>
<td></td>
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<tr>
<td>(16)</td>
<td>4 (0, 0, 1/4) 3/4, z (4z) 3/4, 3/4, 1/4</td>
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</tr>
<tr>
<td>(17)</td>
<td>4 (3/4, 0, 0)</td>
<td>x, 1/2, 1/4 (4x) 1/2, 3/4, 3/4</td>
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<tr>
<td>(18)</td>
<td>2 (0, 1/2, 1/2)</td>
<td>3/8, y+1/4, y (2yz) 3/4, 3/4, 1/4</td>
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<tr>
<td>(19)</td>
<td>2 1/8, y+1/4, y (2yz) 1/4, 1/4, 1/4</td>
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</tr>
<tr>
<td>(20)</td>
<td>4 (1/4, 0, 0) x, 0, 3/4 (4x) 1/4, 3/4, 3/4</td>
<td></td>
</tr>
<tr>
<td>(21)</td>
<td>4 (0, 1/4, 0)</td>
<td>3/4, y, 0 (4y) 3/4, 1/4, 3/4</td>
</tr>
<tr>
<td>(22)</td>
<td>2 (1/2, 0, 1/2)</td>
<td>x−1/4, 3/8, x (2xz) 1/4, 1/4, 3/4</td>
</tr>
<tr>
<td>(23)</td>
<td>4 y (0, 3/4, 0) 1/4, y, 1/2 (4y) 3/4, 3/4, 1/4</td>
<td></td>
</tr>
<tr>
<td>(24)</td>
<td>2 x+1/4, 1/8, x (2xz) 1/4, 1/4, 1/4</td>
<td></td>
</tr>
</tbody>
</table>

For (0, 1/2, 1/2) + set

<table>
<thead>
<tr>
<th>(1)</th>
<th>t (0, 1/2, 1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2)</td>
<td>2 0, 0, z (2z) 0, 0, 0</td>
</tr>
<tr>
<td>(3)</td>
<td>2 1/4, y, 1/4 (2y) 1/2, 1/2, 0</td>
</tr>
<tr>
<td>(4)</td>
<td>2 (1/2, 0, 0) x, 1/4, 0 (2z) 1/2, 1/2, 0</td>
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<tr>
<td>(5)</td>
<td>3 (1/3, 1/3, 1/3) [x−1/3, x−1/6, x (3xyz) 0, 1/2, 1/2]</td>
</tr>
<tr>
<td>(6)</td>
<td>3 x+1/2, x, x (3xyz) 1/2, 2, 1/2</td>
</tr>
<tr>
<td>(7)</td>
<td>3 x, x, x (3xyz) 1/2, 1/2, 0</td>
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<td>(8)</td>
<td>3 x+1/2, x+1/2, x (3xyz) 0, 1/2, 1/2</td>
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<td>(9)</td>
<td>3 (1/3, 1/3, 1/3) [x−1/6, x+1/6, x (3xyz) 0, 1/2, 1/2]</td>
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<td>(10)</td>
<td>3 x+1/2, x, x (3xyz) 1/2, 2, 1/2</td>
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<td>(12)</td>
<td>3 x, x, x (3xyz) 0, 1/2, 1/2</td>
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<tr>
<td>(13)</td>
<td>2 (3/4, 3/4, 0)</td>
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<tr>
<td>(14)</td>
<td>2 [-1/4, 1/4, 0] x, x+1/2, 3/8 (2xy) 1/4, 3/4, 1/4</td>
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<td>(15)</td>
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<td>(16)</td>
<td>4 (0, 0, 3/4) 1/4, 1/2, z (4z) 3/4, 1/4, 3/4</td>
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<tr>
<td>(17)</td>
<td>4 (3/4, 0, 0)</td>
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<td>(18)</td>
<td>2 (0, 1/2, 1/2)</td>
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<td>(19)</td>
<td>2 1/8, y+3/4, y (2yz) 1/4, 3/4, 1/4</td>
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<tr>
<td>(20)</td>
<td>4 (1/4, 0, 0) x, 0, 1/4 (4x) 1/4, 1/4, 1/4</td>
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<tr>
<td>(21)</td>
<td>4 (0, 3/4, 0)</td>
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<td>(22)</td>
<td>2 (1/4, 0, 1/4)</td>
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<td>(23)</td>
<td>4 (0, 1/4, 0) 0, y, 3/4 (4y) 3/4, 1/4, 3/4</td>
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<tr>
<td>(24)</td>
<td>2 [-1/4, 0, 1/4] x+1/2, 3/8, x (2xz) 1/4, 3/4, 1/4</td>
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For (1/2, 0, 1/2) + set

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<td>2 x, 0, 0 (2x) 0, 0, 0</td>
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<tr>
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<td>3 x, x, x (3xyz) 1/2, 2, 1/2</td>
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<tr>
<td>(7)</td>
<td>3 x+1/2, x, x (3xyz) 1/2, 1/2, 0</td>
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<tr>
<td>(8)</td>
<td>3 x, x+1/2, x (3xyz) 0, 1/2, 1/2</td>
</tr>
<tr>
<td>(9)</td>
<td>3 (1/3, 1/3, 1/3) [x−1/6, x+1/6, x (3xyz) 1/2, 0, 1/2]</td>
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<tr>
<td>(10)</td>
<td>3 x, x, x (3xyz) 1/2, 2, 1/2</td>
</tr>
<tr>
<td>(11)</td>
<td>3 x, x, x (3xyz) 0, 1/2, 1/2</td>
</tr>
<tr>
<td>(12)</td>
<td>3 x, x+1/2, x (3xyz) 0, 1/2, 1/2</td>
</tr>
<tr>
<td>(13)</td>
<td>2 (1/4, 1/4, 0)</td>
</tr>
<tr>
<td>(14)</td>
<td>2 (1/4, −1/4, 0) x, x+1/2, 3/8 (2xy) 1/4, 3/4, 1/4</td>
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<tr>
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<td>4 (0, 0, 1/4) 3/4, 0, z (4z) 3/4, 1/4, 3/4</td>
</tr>
<tr>
<td>(16)</td>
<td>4 (0, 0, 3/4) −1/4, 1/2, z (4z) 1/4, 3/4, 3/4</td>
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<tr>
<td>(17)</td>
<td>4 (1/4, 0, 0)</td>
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<tr>
<td>(18)</td>
<td>2 (0, 3/4, 3/4) 1/8, y, y (2yz) 1/4, 3/4, 3/4</td>
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<tr>
<td>(19)</td>
<td>2 (0, −1/4, 1/4) 3/8, y+1/2, y (2yz) 3/4, 1/4, 3/4</td>
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<tr>
<td>(20)</td>
<td>4 (3/4, 0, 0) x, 1/4, 1/2 (4x) 3/4, 3/4, 1/4</td>
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<tr>
<td>(21)</td>
<td>4 (0, 1/4, 0)</td>
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<tr>
<td>(22)</td>
<td>2 (1/2, 0, 1/2)</td>
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<tr>
<td>(23)</td>
<td>4 y (0, 3/4, 0) −1/4, y, 1/2 (4y) 1/4, 3/4, 3/4</td>
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<tr>
<td>(24)</td>
<td>2 x+3/4, 1/8, x (2xz) 3/4, 1/4, 3/4</td>
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</tbody>
</table>
(1) t (1/2,1/2,0) (2) 2 (0,0,1/2) 1/4,0,z (3) 2 0,y,0 (4) 2 x,1/4,1/4
  (1 1/2,1/2,0) (2z 1/2,0,1/2) (2y 0,0,0) (2x 0,1/2,1/2)

(5) 3' (1/3,1/3,1/3) x+1/6,x+1/3,x
  (3xyz 1/2,1/2,0) (3xyz 1/2,1/2,0)

(6) 3' x,x+1/2,x (7) 3' x+1/2,x-1/2,x (8) 3' x,x,x
  (3xyz 1/2,1/2,0) (3xyz 1/2,1/2,1/2) (3xyz 0,0,0)

(9) 3' (1/3,1/3,1/3) x+1/3,x+1/6,x
  (3xyz 1/2,1/2,0) (3xyz 0,0,0)

(10) 3' x,x,x (11) 3' x+1/2,x+1/2,x (12) 3' x,x,x
  (3xyz 1/2,1/2,0) (3xyz 0,0,0) (3xyz 0,0,0)

For (1/2,1/2,0) + set

(1) 1' (0,0,0)' (2) 2' (0,0,1/2) 0,1/4,z (3) 2' (0,1/2,0) 1/4,y,0 (4) 2' (1/2,0,0) x,0,1/4
  (1 0,0,0)' (2z 1/2,1/2,0)' (2y 1/2,1/2,0)' (2x 1/2,1/2,0)'

(5) 3'' x,x,x (6) 3'' (1/3,-1/3,1/3) x+1/6,x+1/6,x
  (3xyz 0,0,0)' (3xyz 1/2,1/2,0)' (3xyz 1/2,1/2,0)'

(7) 3'' (-1/3,1/3,1/3) x+1/3,x-1/6,x (8) 3'' (1/3,1/3,1/3)
  (3xyz 1/2,1/2,1/2) (3xyz 0,0,0)' (3xyz 0,0,0)

(9) 3' x,x,x (10) 3' x,x,x (11) 3' x+1/2,x (12) 3' x,x,x
  (3xyz 1/2,1/2,0) (3xyz 0,0,0) (3xyz 0,1/2,1/2) (3xyz 1/2,0,1/2)

For (0,0,0) + set

(13) 2' (1/2,1/2,0) x,x+1/4,3/8 (14) 2' x,x+1/4,1/8 (15) 4' (0,0,3/4) 1/2,1/4,z (16) 4' (0,0,1/4) 0,1/4,z
  (2zxy 3/4,1/4,3/4)' (2zxy 1/4,1/4,1/4)' (4zxy 1/4,3/4,3/4)'

(17) 4' (3/4,0,0) x,1/2,1/4 (18) 2' (0,1/2,1/2) 3/8,y+1/4,y (19) 2' 1/8,y+1/4,y
  (4zxy 3/4,1/4,3/4) (2zxy 3/4,3/4,1/4)' (2zxy 1/4,1/4,1/4)'

(20) 4' (1/4,0,0) x,0,3/4 (4zxy 1/4,3/4,3/4)'

(21) 4' (0,1/4,0) 3/4,y,0 (22) 2' (1/2,0,1/2) -1/2,3/8,x (23) 4' (0,3/4,0) 1/4,y,1/2
  (4zxy 3/4,1/4,3/4) (2zxy 1/4,3/4,3/4)' (2zxy 1/4,1/4,1/4)'

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2) (2) 2' (0,0,1/2) 0,1/4,z (3) 2' 1/4,y,1/4 (4) 2' (1/2,0,0) x,1/4,0
  (1 0,1/2,1/2)' (2z 0,0,0) (2y 1/2,0,1/2) (2x 1/2,1/2,0)'

(5) 3'' (1/3,1/3,1/3) x-1/3,x-1/6,x
  (3xyz 0,1/2,1/2)' (3xyz 1/2,1/2,2)'

(6) 3'' x+1/2,x,x (7) 3'' x,x,x (8) 3'' x+1/2,x+1/2,x
  (3xyz 1/2,1/2,2)' (3xyz 0,0,0)' (3xyz 0,0,0)

(9) 3' (1/3,1/3,1/3) x-1/6,x+1/6,x
  (3xyz 1/2,1/2,2)' (3xyz 1/2,0,1/2)

(10) 3' x+1/2,x,x (11) 3' x+1/2,x+1/2,x (12) 3' x,x,x
  (3xyz 1/2,0,1/2) (3xyz 1/2,1/2,0)' (3xyz 0,0,0)
Continued

(13) 2' (3/4,3/4,0) x,x,1/8
       (2'xy) 3/4,3/4,1/4)

(14) 2' (-1/4,1/4,0) x,x+1/2,3/8
       (2'xy) 1/4,3/4,3/4)

(15) 4' - (0,0,1/4) 1/4,0,z
       (4'z) 1/4,1/4,1/4)

(16) 4' - (0,0,3/4) 1/4,1/2,z
       (4'z) 3/4,1/4,3/4)

(17) 4' - (3/4,0,0) x,1/2,-1/4
       (4'-xy) 3/4,3/4,1/4)

(18) 2' (0,1/2,1/2) 3/8,y-1/4,y
       (2'xy) 3/4,1/4,3/4)

(19) 2' - (1/2,0,1/2) 1/4,0,z
       (2'xy) 1/4,3/4,3/4)

(20) 4' - (1/4,0,0) x,0,1/4
       (4') 1/4,1,1/4)

(21) 4' - (0,3/4,0) 1/2,y,-1/4
       (4'xy) 3/4,3/4,1/4)

(22) 2' (1/4,0,1/4) x,1/8,x
       (2'xy) 1/4,1/4,1/4)

(23) 4' - (0,1/4,0) 0,y,3/4
       (4'y) 3/4,1/4,3/4)

(24) 2' - (1/4,0,1/4) x,x+1/2,3/8,x
       (2'xy) 1/4,3/4,3/4)

For (1/2,0,1/2) + set

(1) 1' (1/2,0,1/2)
       (1'xy) 1/2,0,1/2)

(2) 2' 1/4,1/4,z
       (2'xy) 1/2,1,2/0,1/2)

(3) 2' (0,1/2,0) 0,y,1/4
       (2'y) 0,1/2,1/2,0)

(4) 2' x,0,0
       (2'z) 0,1/2,1/2,0)

(5) 3' - (1/3,3/1,3/3)

(6) 3' - x,x,x
       (3'xyz) 1/2,0,1/2)

(7) 3' - x+1/2,x,x
       (3'xyz) 1/2,1,2/0,1/2)

(8) 3' - x,x+1/2,x
       (3'xyz) 1/2,0,1/2)

(9) 3' - (1/3,3/1,3/3)

(10) 3' - x,x,x,x+1/6,x
       (3'xyz) 3/4,3/4,1/4)

(11) 3' - x,x,x,x+1/6,x
       (3'xyz) 3/4,3/4,1/4)

(12) 3' - x,x+1/2,x
       (3'xyz) 1/2,0,1/2)

(13) 2' (1/4,1/4,0) x,x,1/8
       (2'xy) 1/4,1/4,1/4)

(14) 2' (1/4,1/4,0) x,x+1/2,3/8
       (2'xy) 3/4,3/4,3/4)

(15) 4' - (0,0,1/4) 3/4,0,z
       (4'z) 1/4,3/4,3/4)

(16) 4' - (0,0,3/4) 1/4,1/2,z
       (4'z) 3/4,1/4,3/4)

(17) 4' - (3/4,0,0) x,1/4,0
       (4'-xy) 3/4,3/4,1/4)

(18) 2' (0,1/4,1/4) 1/8,y,y
       (2'xy) 3/4,3/4,3/4)

(19) 2' (0,1/4,1/4) 3/8,y+1/2,y
       (2'xy) 3/4,3/4,3/4)

(20) 4' - (3/4,0,0) x,1/4,1/2
       (4') 3/4,3/4,1/4)

(21) 4' - (0,3/4,0) 1/2,y,1/4
       (4'xy) 3/4,3/4,1/4)

(22) 2' (3/4,0,3/4) x,1/8,x
       (2'xy) 3/4,3/4,1/4)

(23) 4' - (0,1/4,0) 0,y,1/4
       (4'y) 3/4,1/4,1/4)

(24) 2' (1/4,0,1/4) x,x+1/2,3/8,x
       (2'xy) 3/4,3/4,1/4)

For (1/2,1,2,0) + set

(1) 1' (1/2,1,2,0)
       (1'xy) 1/2,1,2,0)

(2) 2' (0,0,1/2) 1/4,0,z
       (2'xy) 1/2,1,2,0)

(3) 2' (0,0,1/2) 0,y,0
       (2'y) 0,1/2,1/2,0)

(4) 2' x,1/4,1/4
       (2'z) 0,1/2,1/2,0)

(5) 3' - (1/3,3/1,3/3)

(6) 3' - x,x+1/2,x
       (3'xyz) 1/2,1,2,0)

(7) 3' - x,x+1/2,x,x+1/2,x
       (3'xyz) 1/2,1,2,0)

(8) 3' - x,x,x
       (3'xyz) 1/2,1,2,0)

(9) 3' - (1/3,3/1,3/3)

(10) 3' - x,x,x
       (3'xyz) 1/2,1,2,0)

(11) 3' - x,x+1/2,x
       (3'xyz) 1/2,1,2,0)

(12) 3' - x,x+1/2,x,x+1/2,x
       (3'xyz) 1/2,1,2,0)

(13) 2' (1/2,1,2,0) x,x+1/4,3/8
       (2'xy) 1/4,3/4,3/4)

(14) 2' x,x+3/4,1/8
       (2'xy) 3/4,3/4,1/4)

(15) 4' - (0,0,3/4) 1/2,-1/4,z
       (4'z) 3/4,1/4,1/2)

(16) 4' - (0,0,1/4) 0,1/4,z
       (4'z) 1/4,1,1/4)

(17) 4' - (1/4,0,0) x,3/4,0
       (4'-xy) 3/4,3/4,1/4)

(18) 2' (0,1/4,1/4) 1/8,y,y
       (2'xy) 3/4,3/4,1/4)

(19) 2' (0,1/4,1/4) 3/8,y+1/2,y
       (2'xy) 3/4,3/4,1/4)

(20) 4' - (3/4,0,0) x,-1/4,1/2
       (4') 3/4,1,1/4)

(21) 4' - (0,3/4,0) 1/2,y,1/4
       (4'xy) 3/4,3/4,1/4)

(22) 2' (3/4,0,3/4) x,1/8,x
       (2'xy) 3/4,3/4,1/4)

(23) 4' - (0,1/4,0) 0,y,1/4
       (4'y) 3/4,1/4,1/4)

(24) 2' (1/4,0,1/4) x,x+1/2,3/8,x
       (2'xy) 3/4,3/4,1/4)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1,0,1/2); t(1/2,0,1/2); (2); (3); (5); (13): 1'.
Continued

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
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<tr>
<th>Positions</th>
<th>Coordinates</th>
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<td></td>
</tr>
<tr>
<td>96 h 11'</td>
<td></td>
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</tbody>
</table>

(1) x,y,z [0,0,0]  (2) x̅,y̅ +1/2,z̅ +1/2 [0,0,0]  (3) x̅ +1/2,y̅ +1/2,z̅ [0,0,0]  (4) x̅ +1/2,y̅ ,z̅ +1/2 [0,0,0]

(5) z,x,y [0,0,0]  (6) z̅ +1/2,x̅ ,y̅ +1/2 [0,0,0]  (7) z̅ ,x̅ +1/2,y̅ +1/2 [0,0,0]  (8) z̅ +1/2,x̅ +1/2,y̅ [0,0,0]

(9) y,z,x [0,0,0]  (10) y̅ +1/2,z̅ +1/2,x̅ [0,0,0]  (11) y̅ +1/2,z̅ ,x̅ +1/2 [0,0,0]  (12) y̅ ,z̅ +1/2,x̅ +1/2 [0,0,0]

(13) y+3/4,x+1/4,z+3/4 [0,0,0]  (14) y̅ +1/4,x̅ +1/4,z̅ +1/4 [0,0,0]  (15) y̅ +1/4,x̅ +3/4,z̅ +3/4 [0,0,0]  (16) y̅ +3/4,x̅ +3/4,z̅ +1/4 [0,0,0]

(17) x+3/4,z+1/4,y+3/4 [0,0,0]  (18) x̅ +3/4,z̅ +1/4,y̅ +1/4 [0,0,0]  (19) x̅ +1/4,z̅ +1/4,y̅ +1/4 [0,0,0]  (20) x̅ +1/4,z̅ +3/4,y̅ +3/4 [0,0,0]

(21) z+3/4,y+1/4,x+3/4 [0,0,0]  (22) z̅ +1/4,y̅ +3/4,x̅ +1/4 [0,0,0]  (23) z̅ +3/4,y̅ +3/4,x̅ +1/4 [0,0,0]  (24) z̅ +1/4,y̅ +1/4,x̅ +1/4 [0,0,0]

48 g ..21' 1/8, y̅ ,y̅ +1/4 [0,0,0]  7/8, y̅ +1/2, y̅ +3/4 [0,0,0]  3/8, y̅ +1/2, y̅ +3/4 [0,0,0]  5/8, y̅ ,y̅ +1/4 [0,0,0]

48 f 2..1' x, 0,0 [0,0,0]  x̅ ,1/2,1/2 [0,0,0]  0, x, 0 [0,0,0]  1/2, x, 1/2 [0,0,0]

32 e ..3.1' x, x, x [0,0,0]  x̅ , x̅ +1/2,x̅ +1/2 [0,0,0]  x̅ +1/2,x̅ +1/2] [0,0,0]  x̅ +1/2,x̅ +1/2 [0,0,0]

16 d .321' 5/8, 5/8, 5/8 [0,0,0]  3/8, 7/8, 1/8 [0,0,0]  7/8, 1/8, 3/8 [0,0,0]  1/8, 3/8, 7/8 [0,0,0]

16 c .321' 1/8, 1/8, 1/8 [0,0,0]  7/8, 3/8, 5/8 [0,0,0]  3/8, 5/8, 7/8 [0,0,0]  5/8, 7/8, 3/8 [0,0,0]

8 b 23.1' 1/2, 1/2, 1/2 [0,0,0]  1/4, 3/4, 1/4 [0,0,0]

8 a 23.1' 0, 0, 0 [0,0,0]  3/4, 1/4, 3/4 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  Along [1,1,1] p3m11'  Along [1,1,0] c2mm1'

a* = a/2  b* = b/2  a* = (2a - b - c)/6  b* = (-a + 2b - c)/6  a* = (-a + b)/2  b* = c

Origin at 1/4,0,z  Origin at x,x,x  Origin at x,x,1/8
Origin at 3$
$2

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad -1/8 \leq y \leq 1/8; \quad -1/8 \leq z \leq 1/8; \quad y \leq \min(x,1/2-x); \quad -y \leq z \leq \min(x,1/2-x) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/8,1/8,1/8 & \quad 1/8,1/8,-1/8 & \quad 1/8,-1/8,1/8 \\
1/2,0,0 & \quad 3/8,1/8,1/8 & \quad 3/8,1/8,-1/8 & \quad 3/8,-1/8,1/8
\end{align*}
\]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 (0,0,1/2) \quad 0,1/4,z \\
(3) & \quad 2 (0,1/2,0) \quad 1/4,y,0 \\
(4) & \quad 2 (1/2,0,0) \quad x,0,1/4 \\
(5) & \quad 3^+ \quad x,x,x \\
(6) & \quad 3^+ (1/3,-1/3,1/3) \quad x+1/6,x+1/6,x \\
(7) & \quad 3^+ (-1/3,1/3,1/3) \quad x+1/3,x-1/6,x \\
(8) & \quad 3^+ (1/3,1/3,-1/3) \quad x+1/6,x+1/3,x \\
(9) & \quad 3^- \quad x,x,x \\
(10) & \quad 3^- (1/3,-1/3,1/3) \quad x+1/6,x+1/6,x \\
(11) & \quad 3^- (-1/3,1/3,1/3) \quad x+1/3,x-1/6,x \\
(12) & \quad 3^- (1/3,1/3,-1/3) \quad x+1/6,x+1/3,x \\
(3) & \quad 3^- \quad x,x,x \\
(10) & \quad 3^- (1/3,-1/3,1/3) \quad x+1/6,x+1/6,x \\
(11) & \quad 3^- (-1/3,1/3,1/3) \quad x+1/3,x-1/6,x \\
(12) & \quad 3^- (1/3,1/3,-1/3) \quad x+1/6,x+1/3,x \\
(3) & \quad 3^- \quad x,x,x \\
(10) & \quad 3^- (1/3,-1/3,1/3) \quad x+1/6,x+1/6,x \\
(11) & \quad 3^- (-1/3,1/3,1/3) \quad x+1/3,x-1/6,x \\
(12) & \quad 3^- (1/3,1/3,-1/3) \quad x+1/6,x+1/3,x
\end{align*}
\]
Continued 210.3.1555 F4,'32'

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
    (1 | 1/2,1/2,0)  

(2) 2 (0,0,1/2) 1/4,0,z  
    (2_z| 1/2,0,1/2)  

(3) 2 0,y,0  
    (2_y| 0,0,0)  

(4) 2 x,1/4,1/4  
    (2_x| 0,1/2,1/2)  

(5) 3* (1/3,1/3,1/3)  
    x+1/6,x+1/3,x  
    (3_{xyz} | 1/2,1/2,0)  

(6) 3* x,x+1/2,x  
    (3_{xyz}^* | 0,1/2,1/2)  

(7) 3* x+1/2,x+1/2,x+1/2  
    (3_{xyz}^* | 1/2,0,1/2)  

(8) 3* x,x,x  
    (3_{xyz}^* | 0,0,0)  

(9) 3* (1/3,1/3,1/3)  
    x+1/3,x+1/6,x  
    (3_{xyz}^* | 1/2,1/2,0)  

(10) 3* x,x,x  
    (3_{xyz} | 0,0,0)  

(11) 3* x+1/2,x+1/2,x+1/2  
    (3_{xyz} | 0,1/2,1/2)  

(12) 3* (1/3,-1/3,1/3)  
    x-1/6,x+1/3,x  
    (3_{xyz} | 1/2,0,1/2)  

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

96 h 1  

(1) x,y,z [u,v,w]  
    (2) x,x+1/2,z+1/2 [u,v,w]  
    (3) x+1/2,y+1/2,z [u,v,w]  
    (4) x+1/2,y,z+1/2 [u,v,w]  

(5) z,x,y [w,u,v]  
    (6) z+1/2,x,y+1/2 [w,u,v]  
    (7) z,x+1/2,y+1/2 [w,u,v]  
    (8) z+1/2,x+1/2,y [w,u,v]  

(9) y,z,x [v,w,u]  
    (10) y+1/2,z+1/2,x [v,w,u]  
    (11) y+1/2,z,x+1/2 [v,w,u]  
    (12) y,z+1/2,x+1/2 [v,w,u]  

(13) y+3/4,x+1/4,z+3/4 [u,v,w]  
    (14) y+1/4,x+1/4,z+1/4 [v,u,w](15) y+1/4,x+3/4,z+3/4 [v,u,w](16) y+3/4,x+3/4,z+1/4 [v,u,w]  

(17) x+3/4,z+1/4,y+3/4 [u,w,v]  
    (18) x+3/4,z+3/4,y+1/4 [u,w,v]  
    (19) x+1/4,z+1/4,y+1/4 [u,w,v]  
    (20) x+1/4,z+3/4,y+3/4 [u,w,v]  

(21) z+3/4,y+1/4,x+3/4 [w,v,u]  
    (22) z+1/4,y+3/4,x+1/4 [w,v,u]  
    (23) z+3/4,y+3/4,x+1/4 [w,v,u]  
    (24) z+1/4,y+1/4,x+1/4 [w,v,u]  

48 g .2'  

1/8,y+1/4 [u,v,u]  
    y+1/4,1/8 [v,u,v]  
    y+3/4,7/8,y+1/2 [u,v,u]  y+3/4,3/8,y+1/2 [v,u,u] y+1/4,5/8,y [v,u,v]  
    y,y+1/4,1/8 [v,v,u]  

48 f 2.  

x,0,0 [u,v]  
    x,1/2,1/2 [u,0,0]  
    0,x,0 [0,v,0]  
    1/2,x,1/2 [0,0,u]  
    0,0,x [0,0,u]  
    1/2,1/2,x [0,0,u]  
    3/4,x+1/4,3/4 [0,0,u]  
    1/4,x+1/4,1/4 [0,0,u]  
    x+3/4,1/4,3/4 [u,0,0]  
    x+3/4,3/4,1/4 [u,0,0]  
    3/4,1/4,x+3/4 [0,0,u]  
    1/4,3/4,x+3/4 [0,0,u]
Continued

<table>
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<tr>
<th>32</th>
<th>e</th>
<th>0.3</th>
<th>x, x, x [u, u, u]</th>
<th>x, x+1/2, x+1/2 [u, u, u]</th>
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<tr>
<td></td>
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<td></td>
<td>(x + 1/2, x + 1/2, x) [u, u, u]</td>
<td>x + 1/2, x + 1/2 [u, u, u]</td>
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<td></td>
<td></td>
<td>x + 3/4, x + 1/4, x + 3/4 [u, u, u]</td>
<td>x + 1/4, x + 1/4, x + 1/4 [u, u, u]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>x + 1/4, x + 3/4, x + 3/4 [u, u, u]</td>
<td>x + 3/4, x + 3/4, x + 1/4 [u, u, u]</td>
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<table>
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<th>16</th>
<th>d</th>
<th>0.32'</th>
<th>5/8, 5/8, 5/8 [u, u, u]</th>
<th>3/8, 7/8, 1/8 [u, u, u]</th>
<th>7/8, 1/8, 3/8 [u, u, u]</th>
<th>1/8, 3/8, 7/8 [u, u, u]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>8</th>
<th>b</th>
<th>23.</th>
<th>1/2, 1/2, 1/2 [0, 0, 0]</th>
<th>1/4, 3/4, 1/4 [0, 0, 0]</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>0, 0, 0 [0, 0, 0]</td>
<td>3/4, 1/4, 3/4 [0, 0, 0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0, 0, 1] p4'm'm

- \(a^* = a/2\)
- \(b^* = b/2\)
- Origin at 1/4, 0, z

Along [1, 1, 1] p3m1

- \(a^* = (2a - b - c)/6\)
- \(b^* = (-a + 2b - c)/6\)
- Origin at x, x, x

Along [1, 1, 0] c2'm'm'

- \(a^* = c\)
- \(b^* = -(a + b)/2\)
- Origin at x, x, 1/8
Origin at 432

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad z \leq \min(x,1/2-x,y,1/2-y)
\]

Vertices

\[
0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/4,1/4,1/4
\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \ 0,0,z \\
(3) & \quad 2 \ 0,y,0 \\
(4) & \quad 2 \ x,0,0 \\
(5) & \quad 3^+ \ x,x,x \\
(6) & \quad 3^+ \ x,x,x \\
(7) & \quad 3^+ \ x,x,x \\
(8) & \quad 3^+ \ x,x,x \\
(9) & \quad 3^- \ x,x,x \\
(10) & \quad 3^- \ x,x,x \\
(11) & \quad 3^- \ x,x,x \\
(12) & \quad 3^- \ x,x,x \\
\end{align*}
\]
Continued

<table>
<thead>
<tr>
<th>Site Symmetry.</th>
<th>Wyckoff letter,</th>
<th>Multiplicity,</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>(13) 2 x,x,0</td>
<td>(2x) 0,0,0</td>
<td>(2x) 1/2,1/2,1/2</td>
<td>(2x) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(14) 2 x,x,0</td>
<td>(2y) 0,0,0</td>
<td>(2y) 1/2,1/2,1/2</td>
<td>(2y) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(15) 4' 0,0,z</td>
<td>(4z) 0,0,0</td>
<td>(4z) 0,0,0</td>
<td>(4z) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(16) 4' 0,0,z</td>
<td>(4z) 0,0,0</td>
<td>(4z) 0,0,0</td>
<td>(4z) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(17) 4' x,0,0</td>
<td>(4z) 0,0,0</td>
<td>(4z) 1/2,1/2,1/2</td>
<td>(4z) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(18) 2 y,y,y</td>
<td>(2yz) 0,0,0</td>
<td>(2yz) 0,0,0</td>
<td>(2yz) 0,0,0</td>
</tr>
<tr>
<td>(19) 2 y,y,y</td>
<td>(2yz) 0,0,0</td>
<td>(2yz) 0,0,0</td>
<td>(2yz) 0,0,0</td>
</tr>
<tr>
<td>(20) 4' x,0,0</td>
<td>(4z) 0,0,0</td>
<td>(4z) 0,0,0</td>
<td>(4z) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(21) 4' y,0,0</td>
<td>(4y) 0,0,0</td>
<td>(4y) 0,0,0</td>
<td>(4y) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(22) 2 x,0,x</td>
<td>(2xz) 0,0,0</td>
<td>(2xz) 0,0,0</td>
<td>(2xz) 0,0,0</td>
</tr>
<tr>
<td>(23) 4' y,0,0</td>
<td>(4y) 0,0,0</td>
<td>(4y) 0,0,0</td>
<td>(4y) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(24) 2 y,0,x</td>
<td>(4y) 0,0,0</td>
<td>(4y) 0,0,0</td>
<td>(4y) 1/2,1/2,1/2</td>
</tr>
</tbody>
</table>

For (1/2,1/2,1/2) + set

<table>
<thead>
<tr>
<th>Site Symmetry.</th>
<th>Wyckoff letter,</th>
<th>Multiplicity,</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (1/2,1/2,1/2)</td>
<td>(2x) 0,0,0</td>
<td>(2x) 1/2,1/2,1/2</td>
<td>(2x) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(1) (1/2,1/2,1/2)</td>
<td>(2x) 0,0,0</td>
<td>(2x) 1/2,1/2,1/2</td>
<td>(2x) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(5) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(6) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(7) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(8) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(9) 3' (1/2,1/2,1/2) x,x,x</td>
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<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(10) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(11) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(12) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(13) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(14) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(15) 3' (1/2,1/2,1/2) x,x,x</td>
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<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
</tr>
<tr>
<td>(16) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(17) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
<td>(3x) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>(18) 3' (1/2,1/2,1/2) x,x,x</td>
<td>(3x) 1/2,1/2,1/2</td>
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<tr>
<td>(19) 3' (1/2,1/2,1/2) x,x,x</td>
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<td>(20) 3' (1/2,1/2,1/2) x,x,x</td>
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<tr>
<td>(21) 3' (1/2,1/2,1/2) x,x,x</td>
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<tr>
<td>(22) 3' (1/2,1/2,1/2) x,x,x</td>
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<td>(3x) 1/2,1/2,1/2</td>
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<td>(23) 3' (1/2,1/2,1/2) x,x,x</td>
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<td>(24) 3' (1/2,1/2,1/2) x,x,x</td>
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</table>

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

211.1.1556 - 2 - 3497
Symmetry of Special Projections

Along [0,0,1] p4m'm'

\[ a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \]

Origin at 0,0,z

Along [1,1,1] p3m'1

\[ a^* = \frac{(2a - b - c)}{3} \quad b^* = \frac{(a + 2b - c)}{3} \]

Origin at x,x,x

Along [1,1,0] p2m'm'

\[ a^* = \frac{-(a + b)}{2} \quad b^* = \frac{c}{2} \]

Origin at x,x,0

---

24 i .2 1/4,y,\(y+1/2\) [0,v,v] 3/4,y,\(y+1/2\) [0,v,v] 3/4,y,\(y+1/2\) [0,v,v] 1/4,y,\(y+1/2\) [0,v,v] \\
\(y+1/2,3/4\) [v,v,0] \(y+1/2,3/4\) [v,v,0] \(y+1/2,3/4\) [v,v,0] \(y+1/2,3/4\) [v,v,0] \\
\(y,\overline{y}+1/2,1/4\) [v,v,0] \(\overline{y},\overline{y}+1/2,1/4\) [v,v,0] \(\overline{y},\overline{y}+1/2,1/4\) [v,v,0] \(\overline{y},\overline{y}+1/2,1/4\) [v,v,0]

24 h .2 0,y,\(0,0\) 0,y,\(0,0\) 0,y,\(0,0\) 0,y,\(0,0\) \\
y,0,y [v,0,v] \(\overline{y},0,y[v,0,v]\) \(\overline{y},0,y[v,0,v]\) \(\overline{y},0,y[v,0,v]\) \\
y,0,y [v,0,v] \(\overline{y},0,y[v,0,v]\) \(\overline{y},0,y[v,0,v]\) \(\overline{y},0,y[v,0,v]\)

24 g 2.. 1/2,0,x [0,0,u] 0,1/2,0 [0,0,u] 0,1/2,0 [0,0,u] 0,1/2,0 [0,0,u] \\
1/2,0,x [0,0,u] \(\overline{x},1/2,0\) [\(\overline{u},0,0\)] \(\overline{x},1/2,0\) [\(\overline{u},0,0\)] \(\overline{x},1/2,0\) [\(\overline{u},0,0\)] \\
x,0,1/2 [0,0,u] \(\overline{x},0,1/2\) [\(\overline{u},0,0\)] \(\overline{x},0,1/2\) [\(\overline{u},0,0\)] \(\overline{x},0,1/2\) [\(\overline{u},0,0\)]

16 f .3. x,x,x [u,u,u] \(\overline{x},\overline{x},x[u,u,u]\) \(\overline{x},\overline{x},x[u,u,u]\) \(\overline{x},\overline{x},x[u,u,u]\) \\
x,x,x [u,u,u] \(\overline{x},\overline{x},x[u,u,u]\) \(\overline{x},\overline{x},x[u,u,u]\) \(\overline{x},\overline{x},x[u,u,u]\)

12 e 4.. x,0,0 [u,0,0] \(\overline{x},0,0 [\overline{u},0,0]\) \(\overline{x},0,0 [\overline{u},0,0]\) \(\overline{x},0,0 [\overline{u},0,0]\) \\
0,x,0 [0,0,u] 0,0,x [0,0,u] 0,0,x [0,0,u] 0,0,x [0,0,u] \\
12 d 2.22 1/4,1/2,0 [0,0,0] 3/4,1/2,0 [0,0,0] 0,1/4,1/2 [0,0,0] \\
0,3/4,1/2 [0,0,0] \(1/2,0,1/4\) [0,0,0] \(1/2,0,1/4\) [0,0,0] \(1/2,0,1/4\) [0,0,0]

8 c .32 1/4,1/4,1/4 [0,0,0] 3/4,3/4,1/4 [0,0,0] 3/4,1/4,3/4 [0,0,0] 1/4,3/4,3/4 [0,0,0] \\
6 b 42.2 0,1/2,1/2 [0,0,0] \(1/2,0,1/2\) [0,0,0] \(1/2,1/2,0\) [0,0,0] \\
2 a 432 0,0,0 [0,0,0] 

211.1.1556 - 3 - 3498
I4321' Cubic
211.2.1557 I4321'

Origin at 432
Asymmetric unit
0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; z \leq \min(x, 1/2-x, y, 1/2-y)

Vertices
0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/4,1/4,1/4

Symmetry Operations
For (0,0,0) + set

(1) 1
(1) 0,0,0
(1) 0,0,0

(2) 2 0,0,z
(2) 0,0,0
(2) 0,0,0

(3) 2 y,0,0
(3) 0,0,0
(3) 0,0,0

(4) 2 x,0,0
(4) 0,0,0
(4) 0,0,0

(5) 3^+ x,x,x
(3_{xyz}^{-1} 0,0,0)

(6) 3^+ x,x,x
(3_{xyz}^{-1} 0,0,0)

(7) 3^+ x,x,x
(3_{xyz}^{-1} 0,0,0)

(8) 3^- x,x,x
(3_{xyz}^{-1} 0,0,0)

(9) 3^- x,x,x
(3_{xyz}^{-1} 0,0,0)

(10) 3^- x,x,x
(3_{xyz}^{-1} 0,0,0)

(11) 3^- x,x,x
(3_{xyz}^{-1} 0,0,0)

(12) 3^- x,x,x
(3_{xyz}^{-1} 0,0,0)
(13) 2 x,x,0
(2xy 0,0,0)

(14) 2 x,x,0
(2xy 0,0,0)

(15) 4' 0,0,0 z
(4z 0,0,0)

(16) 4* 0,0,0
(4z 0,0,0)

(17) 4* x,0,0
(4' z 0,0,0)

(18) 2 0,y,0
(2yz 0,0,0)

(19) 2 0,y,0
(2yz 0,0,0)

(20) 4* x,0,0
(4z 0,0,0)

(21) 4* y,0,0
(4y 0,0,0)

(22) 2 x,0,x
(2xz 0,0,0)

(23) 4* y,0,0
(4y 0,0,0)

(24) 2* x,0,0
(2xz 0,0,0)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(2) 2 (0,0,1/2) 1/4,1/4,z
(3) 2 (0,1/2,0) 1/4,y,1/4
(4) 2 (1/2,0,0) x,1/4,1/4

(2) 2 (1/2,1/2,1/2)

(3) 2 (1/2,1/2,1/2)
(4) 2 (1/2,1/2,1/2)

(5) 3* (1/2,1/2,1/2) x,x,x
(6) 3* (1/6,-1/6,1/6)

(7) 3* (-1/6,1/6,1/6)

(8) 3* (1/6,1/6,-1/6)

(2) x,x,0
(8) 2 0,y,0

(9) 3' (1/2,1/2,1/2) x,x,x
(10) 3' (-1/6,1/6,1/6)

(11) 3' (1/6,1/6,-1/6)

(12) 3' (1/6,-1/6,1/6)

(3xyz -1 1/2,1/2,1/2)

(4z 1/2,1/2,1/2)

(2) x,x,0
(8) 2 0,y,0

(13) 2 (1/2,1/2,0) x,x,1/4
(2xy 1/2,1/2,1/2)

(14) 2 x,x+1/2,1/4
(2y 1/2,1/2,1/2)

(15) 4* (0,0,1/2) 1/2,0,z
(4z 1/2,1/2,1/2)

(16) 4* (0,1/2,0) 1/2,0,z
(4z 1/2,1/2,1/2)

(17) 4* (1/2,0,0) x,1/2,0
(4x -1 1/2,1/2,1/2)

(18) 2 (0,1/2,1/2) 1/4,y,y
(2yz 1/2,1/2,1/2)

(19) 2 1/4,y+1/2,y
(2yz 1/2,1/2,1/2)

(20) 4* (1/2,0,0) x,0,1/2
(4z 1/2,1/2,1/2)

(21) 4* (0,1/2,0) 1/2,y,0
(4y 1/2,1/2,1/2)

(22) 2 (1/2,0,1/2) x,1/4,x
(2xz 1/2,1/2,1/2)

(23) 4* (0,1/2,0) 0,y,1/2
(4y -1 1/2,1/2,1/2)

(24) 2* x+1/2,1/4,x
(2xz 1/2,1/2,1/2)

For (0,0,0)' + set

(1) 1'
(1* 0,0,0)

(2) 2' 0,0,0
(2z 0,0,0)

(3) 2' 0,y,0
(2y 0,0,0)

(4) 2' x,0,0
(2x 0,0,0)

(5) 3* x,x,x
(3xyz 0,0,0)

(6) 3* x,x,x
(3xyz -1 0,0,0)

(7) 3* x,x,x
(3xyz -1 0,0,0)

(8) 3* x,x,x
(3xyz -1 0,0,0)

(9) 3' x,x,x
(3xyz 0,0,0)

(10) 3' x,x,x
(3xyz 0,0,0)

(11) 3' x,x,x
(3xyz 0,0,0)

(12) 3' x,x,x
(3xyz 0,0,0)

(13) 2' x,x,0
(2xy 0,0,0)

(14) 2' x,x,0
(2xy 0,0,0)

(15) 4* 0,0,0
(4z 0,0,0)

(16) 4* 0,0,0
(4z 0,0,0)

(17) 4* x,0,0
(4x -1 0,0,0)

(18) 2' 0,y,0
(2yz 0,0,0)

(19) 2' 0,y,0
(2yz 0,0,0)

(20) 4* x,0,0
(4z 0,0,0)

(21) 4* y,0,0
(4y 0,0,0)

(22) 2' x,0,x
(2xz 0,0,0)

(23) 4* y,0,0
(4y 0,0,0)

(24) 2* x,0,x
(2xz 0,0,0)
Continued

For \((1/2,1/2,1/2)^{\prime}\) + set

\((1)\) \(t^{\prime}(1/2,1/2,1/2)\)
\((2)\) \(2^{\prime}(0,0,1/2)\) \(1/4,1/4,z\)
\((3)\) \(2^{\prime}(0,1/2,0)\) \(1/4,y,1/4\)
\((4)\) \(2^{\prime}(1/2,0,0)\) \(x,1/4,1/4\)
\((5)\) \(3^{\prime} (1/2,1/2,1/2)\) \(x,x,x\)
\((6)\) \(3^{\prime} (1/6,-1/6,1/6)\) \(x+1/3,x+1/3,x\)
\((7)\) \(3^{\prime} (-1/6,1/6,-1/6)\) \(x+2/3,x+1/3,x\)
\((8)\) \(3^{\prime} (1/6,1/6,-1/6)\) \(x+1/3,x+2/3,x\)
\((9)\) \(3^{\prime} (1/2,1/2,1/2)\) \(x,x,x\)
\((10)\) \(3^{\prime} (-1/6,1/6,1/6)\) \(x+1/3,x+1/3,x\)
\((11)\) \(3^{\prime} (1/6,1/6,-1/6)\) \(x+2/3,x+1/3,x\)
\((12)\) \(3^{\prime} (1/6,-1/6,1/6)\) \(x-1/3,x+2/3,x\)
\((13)\) \(2^{\prime} (1/2,1/2,0)\) \(x,x,1/4\)
\((14)\) \(2^{\prime} (0,1/2,1/2)\) \(1/2,0,z\)
\((15)\) \(4^{\prime} (0,0,1/2)\) \(1/2,0,z\)
\((16)\) \(4^{\prime} (0,1/2,1/2)\) \(x,1/4,1/4\)
\((17)\) \(4^{\prime} (1/2,0,0)\) \(x,1/2,1/2\)
\((18)\) \(2^{\prime} (1/2,1/2,0)\) \(1/4,y,y\)
\((19)\) \(2^{\prime} (1/2,1/2,0)\) \(1/4,y+1/2,y\)
\((20)\) \(4^{\prime} (1/2,0,0)\) \(x,1/2,1/2\)
\((21)\) \(4^{\prime} (0,1/2,0)\) \(x,1/4,4\)
\((22)\) \(4^{\prime} (0,1/2,0)\) \(1/2,0,z\)
\((23)\) \(4^{\prime} (0,1/2,0)\) \(1/4,y,1/4\)
\((24)\) \(4^{\prime} (1/2,1/2,0)\) \(1/4,y+1/2,1/4\)

Generators selected
(1); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(1/2,1/2,1/2)\);
(2); (3); (5); (13); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>(0,0,0) +</td>
</tr>
<tr>
<td></td>
<td>(0,0,0)' +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td>(1/2,1/2,1/2)' +</td>
</tr>
</tbody>
</table>

| (1) | x,y,z [0,0,0] |
| (2) | \(\bar{x},\bar{y},\bar{z} [0,0,0]\) |
| (3) | \(\bar{x},\bar{y},\bar{z} [0,0,0]\) |
| (4) | \(x,\bar{y},\bar{z} [0,0,0]\) |
| (5) | z,x,y [0,0,0] |
| (6) | \(z,\bar{x},\bar{y} [0,0,0]\) |
| (7) | \(\bar{z},\bar{x},y [0,0,0]\) |
| (8) | \(z,x,\bar{y} [0,0,0]\) |
| (9) | y,z,x [0,0,0] |
| (10) | \(y,\bar{z},\bar{x} [0,0,0]\) |
| (11) | \(\bar{y},\bar{z},x [0,0,0]\) |
| (12) | \(y,\bar{z},x [0,0,0]\) |
| (13) | y,z,\(\bar{z} [0,0,0]\) |
| (14) | \(y,\bar{x},\bar{z} [0,0,0]\) |
| (15) | \(y,\bar{x},\bar{z} [0,0,0]\) |
| (16) | \(\bar{y},x,z [0,0,0]\) |
| (17) | x,z,\(\bar{y} [0,0,0]\) |
| (18) | \(\bar{x},z,\bar{y} [0,0,0]\) |
| (19) | \(\bar{x},\bar{z},y [0,0,0]\) |
| (20) | \(x,\bar{z},y [0,0,0]\) |
| (21) | z,y,\(\bar{z} [0,0,0]\) |
| (22) | \(z,\bar{y},x [0,0,0]\) |
| (23) | \(\bar{z},\bar{y},x [0,0,0]\) |
| (24) | \(\bar{z},\bar{y},x [0,0,0]\) |

211.2.1557 - 3 - 3501
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>24 h</strong></td>
<td>0.21'</td>
<td>0, y, [0, 0, 0]</td>
</tr>
<tr>
<td></td>
<td>0, y, y, [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0, y, y, y, [0, 0, 0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0, y, 0, 0, 0, 0</td>
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<tr>
<td></td>
<td>0, y, 0, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>y, 0, 0, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td><strong>24 g</strong></td>
<td>0.21'</td>
<td>x, 1/2, 0, [0, 0, 0]</td>
</tr>
<tr>
<td></td>
<td>x, 1/2, 0, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x, 1/2, 0, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td><strong>16 f</strong></td>
<td>0.31'</td>
<td>x, x, x, 0, 0, 0</td>
</tr>
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<td></td>
<td>x, x, x, 0, 0, 0</td>
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<tr>
<td></td>
<td>x, x, x, 0, 0, 0</td>
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<tr>
<td></td>
<td>x, x, x, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td><strong>12 e</strong></td>
<td>0.41'</td>
<td>x, 0, 0, 0, 0, 0</td>
</tr>
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<td></td>
<td>x, 0, 0, 0, 0, 0</td>
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<tr>
<td></td>
<td>x, 0, 0, 0, 0, 0</td>
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</tr>
<tr>
<td><strong>12 d</strong></td>
<td>2.221'</td>
<td>0.34, 1/2, 0, 0, 0, 0</td>
</tr>
<tr>
<td></td>
<td>0.34, 1/2, 0, 0, 0, 0</td>
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<tr>
<td></td>
<td>0.34, 1/2, 0, 0, 0, 0</td>
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</tr>
<tr>
<td><strong>8 c</strong></td>
<td>0.321'</td>
<td>3.43, 1/4, 1/4, 0, 0, 0</td>
</tr>
<tr>
<td></td>
<td>3.43, 1/4, 1/4, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.43, 1/4, 1/4, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td><strong>6 b</strong></td>
<td>4.21'</td>
<td>1/2, 0, 1/2, 0, 0, 0</td>
</tr>
<tr>
<td></td>
<td>1/2, 0, 1/2, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1/2, 0, 1/2, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td><strong>2 a</strong></td>
<td>4321'</td>
<td>0, 0, 0, 0, 0, 0</td>
</tr>
<tr>
<td></td>
<td>0, 0, 0, 0, 0, 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0, 0, 0, 0, 0, 0</td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0, 0, 1] p4mm1'  
\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]  
Origin at 0, 0, z  
Along [1, 1, 1] p3m11'  
\[ \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \quad \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3 \]  
Origin at x, x, x  
Along [1, 1, 0] p2mm1'  
\[ \mathbf{a}^* = (\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]  
Origin at x, x, 0
**Origin** at 4'32'

**Asymmetric unit**

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad z \leq \min(x,1/2-x,y,1/2-y) \]

**Vertices**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0,0,0</td>
<td>1/2,0,0</td>
<td>1/2,1/2,0</td>
</tr>
</tbody>
</table>

**Symmetry Operations**

For \((0,0,0) + \text{ set}\)

1. \(1\)
   
2. \(2 \ 0,0,z\)  
   \(2 \ 0,0,0\)

3. \(2 \ 0,y,0\)  
   \(2 \ 0,0,0\)

4. \(2 \ x,0,0\)  
   \(2 \ 0,0,0\)

5. \(3^+ \ x,x,x\)  
   \((3_{xyz} \ | \ 0,0,0)\)

6. \(3^+ \ x,x,x\)  
   \((3_{xyz}^{-1} \ | \ 0,0,0)\)

7. \(3^+ \ x,x,x\)  
   \((3_{xyz}^{-1} \ | \ 0,0,0)\)

8. \(3^+ \ x,x,x\)  
   \((3_{xyz}^{-1} \ | \ 0,0,0)\)

9. \(3^- \ x,x,x\)  
   \((3_{xyz} \ | \ 0,0,0)\)

10. \(3^- \ x,x,x\)  
    \((3_{xyz}^{-1} \ | \ 0,0,0)\)

11. \(3^- \ x,x,x\)  
    \((3_{xyz} \ | \ 0,0,0)\)

12. \(3^- \ x,x,x\)  
    \((3_{xyz}^{-1} \ | \ 0,0,0)\)
Continued

(13) $2'\ x,x,0$
(21) $4'\ x,y,0$
(17) $4'\ x,0,0$
(20) $x+y,0$
(14) $2'\ x,0,0$
(18) $2'\ 0,y,0$
(19) $2'\ 0,y,0$
(22) $2'\ x,0,0$
(15) $4'\ 0,0,z$
(19) $2'\ 0,y,0$
(23) $4'\ 0,y,0$
(16) $4'\ 0,0,z$
(24) $2'\ x,0,0$
(25) $4'\ 0,0,0$

For $(1/2,1/2,1/2) +$ set

(1) $t(1/2,1/2,1/2)$
(5) $3^+ (1/2,1/2,1/2)$
(9) $3^- (1/2,1/2,1/2)$
(13) $2' (1/2,1/2,0)$
(17) $4' (1/2,0,0)$
(21) $4' (0,1/2,0)$

Generators selected
(1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(1/2,1/2,1/2)$; (2); (3); (5); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Coordinates

$(0,0,0) + \frac{1}{2},1/2,1/2 +$

48 j 1

(1) $x,y,z [u,v,w]$
(5) $z,x,y [w,u,v]$
(9) $y,z,x [v,w,u]$
(13) $y,x,z [\bar{v},\bar{u},w]$
(17) $x,z,y [u,w,v]$
(21) $z,y,x [w,v,u]$

(2) $\bar{x},y,z [\bar{u},\bar{v},w]$
(6) $z,x,y [w,u,v]$
(10) $\bar{y},z,x [\bar{v},\bar{w},u]$
(14) $\bar{y},x,z [\bar{v},\bar{w},u]$
(18) $x,z,y [u,w,v]$
(22) $z,y,x [w,v,u]$

(3) $x,y,z [u,v,w]$
(7) $\bar{z},x,y [\bar{v},\bar{u},v]$
(11) $\bar{y},z,x [\bar{v},\bar{w},u]$
(15) $y,x,z [v,u,w]$
(19) $x,z,y [u,w,v]$
(23) $\bar{z},y,x [w,v,u]$

(4) $x,y,z [u,v,w]$
(8) $\bar{z},x,y [\bar{v},\bar{u},v]$
(12) $\bar{y},z,x [\bar{v},\bar{w},u]$
(16) $y,x,z [v,u,w]$
(20) $x,z,y [u,w,v]$
(24) $\bar{z},y,x [w,v,u]$
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>24</td>
<td>i</td>
<td>.2'</td>
<td>1/4, y, y + 1/2 [u, v, v]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4, y, y + 1/2 [u, v, v]</td>
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<td>3/4, y, y + 1/2 [u, v, v]</td>
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<td>1/4, y, y + 1/2 [u, v, v]</td>
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<td>y + 1/2, 1/4 [v, u, v]</td>
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<td>y + 1/2, 1/4 [v, u, v]</td>
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<td>y + 1/2, 1/4 [v, u, v]</td>
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<td>y + 1/2, 1/4 [v, u, v]</td>
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<tr>
<td>24</td>
<td>h</td>
<td>.2'</td>
<td>0, y, y [u, v, v]</td>
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<td>0, y, y [u, v, v]</td>
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<td>0, y, y [u, v, v]</td>
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<td>0, y, y [u, v, v]</td>
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<tr>
<td>24</td>
<td>g</td>
<td>2.'</td>
<td>x, 1/2, 0 [u, 0, 0]</td>
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<td>x, 1/2, 0 [u, 0, 0]</td>
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<td>x, x, x [u, u, u]</td>
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<td>x, x, x [u, u, u]</td>
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<tr>
<td>12</td>
<td>e</td>
<td>4.'</td>
<td>x, 0, 0 [u, 0, 0]</td>
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<td>x, 0, 0 [u, 0, 0]</td>
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<tr>
<td>12</td>
<td>d</td>
<td>2.'</td>
<td>1/4, 1/2, 0 [u, 0, 0]</td>
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<td>3/4, 1/2, 0 [u, 0, 0]</td>
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<td>3/4, 1/2, 0 [u, 0, 0]</td>
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<td>3/4, 1/2, 0 [u, 0, 0]</td>
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<tr>
<td>8</td>
<td>c</td>
<td>.3'</td>
<td>1/4, 1/4, 1/4 [u, u, u]</td>
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<td>3/4, 3/4, 1/4 [u, u, u]</td>
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<td>3/4, 3/4, 1/4 [u, u, u]</td>
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<td>3/4, 3/4, 1/4 [u, u, u]</td>
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<td>3/4, 3/4, 1/4 [u, u, u]</td>
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<tr>
<td>6</td>
<td>b</td>
<td>4.'</td>
<td>0, 1/2, 1/2 [0, 0, 0]</td>
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<td></td>
<td></td>
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<td>1/2, 0, 1/2 [0, 0, 0]</td>
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<td>1/2, 0, 1/2 [0, 0, 0]</td>
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<td>1/2, 0, 1/2 [0, 0, 0]</td>
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<td>1/2, 0, 1/2 [0, 0, 0]</td>
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<td>2</td>
<td>a</td>
<td>4.'</td>
<td>0, 0, 0 [0, 0, 0]</td>
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<td>0, 0, 0 [0, 0, 0]</td>
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<td>0, 0, 0 [0, 0, 0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0, 0, 1] p4'mm'

<table>
<thead>
<tr>
<th>a*</th>
<th>b*</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a - b)/2</td>
<td>(a + b)/2</td>
</tr>
</tbody>
</table>

Origin at 0, 0, z

Along [1, 1, 1] p3m1

<table>
<thead>
<tr>
<th>a*</th>
<th>b*</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2a - b - c)/3</td>
<td>(-a + 2b - c)/3</td>
</tr>
</tbody>
</table>

Origin at x, x, x

Along [1, 1, 0] p2'mm'

<table>
<thead>
<tr>
<th>a*</th>
<th>b*</th>
</tr>
</thead>
<tbody>
<tr>
<td>c/2</td>
<td>-(a + b)/2</td>
</tr>
</tbody>
</table>

Origin at x, x, 0
Origin at 432

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad z \leq \min(x,1/2-x,y,1/2-y) \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/4,1/4,1/4 \]

Symmetry Operations

For \((0,0,0) + \) set

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 0,0,z \\
(2) & \quad (0,0,0) \\
(3) & \quad 0,y,0 \\
(3) & \quad (0,0,0) \\
(4) & \quad x,0,0 \\
(4) & \quad (0,0,0) \\
(5) & \quad 3^+ \ x,x,x \\
(5) & \quad (3_{xyz} \ | 0,0,0) \\
(6) & \quad x,x,x \\
(6) & \quad (3_{xyz}^{-1} \ | 0,0,0) \\
(7) & \quad 3^+ \ x,x,x \\
(7) & \quad (3_{xyz}^{-1} \ | 0,0,0) \\
(8) & \quad 3^+ \ x,x, \ x \\
(8) & \quad (3_{xyz}^{-1} \ | 0,0,0) \\
(9) & \quad 3^+ \ x,x,x \\
(9) & \quad (3_{xyz}^{-1} \ | 0,0,0) \\
(10) & \quad 3^+ \ x,x, \ x \\
(10) & \quad (3_{xyz}^{-1} \ | 0,0,0) \\
(11) & \quad 3^+ \ x,x, \ x \\
(11) & \quad (3_{xyz}^{-1} \ | 0,0,0) \\
(12) & \quad 3^+ \ x,x, \ x \\
(12) & \quad (3_{xyz}^{-1} \ | 0,0,0) \\
\end{align*}
Continued

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>j</td>
<td>1</td>
</tr>
</tbody>
</table>

(0,0,0) + (1/2,1/2,1/2)’ + set

1. t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

For (1/2,1/2,1/2)’ + set

1. t(1/2,1/2,1/2)
2. 2’ (0,0,1/2) 1/4,1/4,1/4 (2xy) 1/2,1/2,1/2’
3. 2’ (0,1/2,0) 1/4,y,1/4 (2xz) 1/2,1/2,1/2’
4. 2’ (1/2,0,0) x,1/4,1/4 (2yz) 1/2,1/2,1/2’

5. 3* ’ (1/2,1/2,1/2) x,x,x
6. 3* ’ (1/2,1/2,1/2) x,x,x
7. 3* ’ (1/2,1/2,1/2) x,x,x
8. 3* ’ (1/2,1/2,1/2) x,x,x

9. 3’ (1/2,1/2,1/2) x,x,x
10. 3’ (1/2,1/2,1/2) x,x,x
11. 3’ (1/2,1/2,1/2) x,x,x
12. 3’ (1/2,1/2,1/2) x,x,x

13. 2’ (1/2,1/2,1/2) x,x,1/4 (2xz) 1/2,1/2,1/2’
14. 2’ (1/2,1/2,1/2) x,x,1/4 (2xz) 1/2,1/2,1/2’
15. 4 ’ (0,0,1/2) 1/2,0,1/2 (2yz) 1/2,1/2,1/2’
16. 4 ’ (0,0,1/2) 1/2,0,1/2 (2yz) 1/2,1/2,1/2’

17. 4’ (1/2,0,0) x,1/2,0 (2xy) 1/2,1/2,1/2’
18. 2’ (0,1/2,1/2) 1/4,y,y (2yz) 1/2,1/2,1/2’
19. 2’ (0,1/2,1/2) 1/4,y,y (2yz) 1/2,1/2,1/2’
20. 4’ (1/2,0,0) x,0,1/2 (2xz) 1/2,1/2,1/2’

21. 4’ (0,1/2,0) 1/2,y,0 (2xz) 1/2,1/2,1/2’
22. 2’ (1/2,0,1/2) x,1/4,x (2xz) 1/2,1/2,1/2’
23. 4’ (0,1/2,0) 0,y,1/2 (2xz) 1/2,1/2,1/2’
24. 2’ x+1/2,1/4,x (2xz) 1/2,1/2,1/2’

25. 3+ (1/2,1/2,1/2) x,x,x (2xy) 1/2,1/2,1/2’
26. 3+ (1/2,1/2,1/2) x,x,x (2xy) 1/2,1/2,1/2’
27. 3+ (1/2,1/2,1/2) x,x,x (2xy) 1/2,1/2,1/2’
28. 3+ (1/2,1/2,1/2) x,x,x (2xy) 1/2,1/2,1/2’

29. 2 - x,x,0 (2xz) 0,0,0,0 (2yz) 0,0,0,0
30. 2 - x,x,0 (2xz) 0,0,0,0 (2yz) 0,0,0,0
31. 2 - x,x,0 (2xz) 0,0,0,0 (2yz) 0,0,0,0
32. 2 - x,x,0 (2xz) 0,0,0,0 (2yz) 0,0,0,0

33. 4’ 0,0,z (4z) 0,0,0,0
34. 4’ 0,0,z (4z) 0,0,0,0
35. 4’ 0,0,z (4z) 0,0,0,0
36. 4’ 0,0,z (4z) 0,0,0,0

37. 4 - 0,0,z (4z) 0,0,0,0
38. 4 - 0,0,z (4z) 0,0,0,0
39. 4 - 0,0,z (4z) 0,0,0,0
40. 4 - 0,0,z (4z) 0,0,0,0

41. 4+ 0,0,z (4z) 0,0,0,0
42. 4+ 0,0,z (4z) 0,0,0,0
43. 4+ 0,0,z (4z) 0,0,0,0
44. 4+ 0,0,z (4z) 0,0,0,0

45. 4 - 0,0,z (4z) 0,0,0,0
46. 4 - 0,0,z (4z) 0,0,0,0
47. 4 - 0,0,z (4z) 0,0,0,0
48. 4 - 0,0,z (4z) 0,0,0,0
### Symmetry of Special Projections

#### Origin at 0,0,z

<table>
<thead>
<tr>
<th>Along [1,0,0]</th>
<th>a' = (a - b)/2</th>
<th>b' = (a + b)/2</th>
<th>Origin at 0,0,2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,1,0]</td>
<td>a' = c/2</td>
<td>b' = -(a + b)/2</td>
<td>Origin at x,x,0</td>
</tr>
<tr>
<td>Along [1,1,1]</td>
<td>p3m11'</td>
<td>b = (a - 2b - c)/3</td>
<td>Origin at x,x,x</td>
</tr>
</tbody>
</table>

#### Origin at x,x,x

<table>
<thead>
<tr>
<th>Along [1,0,1]</th>
<th>a' = (a - b)/2</th>
<th>b' = (a + b)/2</th>
<th>Origin at 0,0,1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,1,1]</td>
<td>p4mm'</td>
<td>b = (a + b)/2</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

#### Origin at x,x,0

<table>
<thead>
<tr>
<th>Along [1,0,1]</th>
<th>a' = (a + b)/2</th>
<th>b' = (a - b)/2</th>
<th>Origin at 0,0,1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,1,1]</td>
<td>p2m1</td>
<td>b = (a - b)/2</td>
<td>Origin at x,x,0</td>
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#### Origin at x,x,x

<table>
<thead>
<tr>
<th>Along [1,0,1]</th>
<th>a' = (a + b)/2</th>
<th>b' = (a - b)/2</th>
<th>Origin at 0,0,1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [1,1,1]</td>
<td>p4mm'</td>
<td>b = (a - b)/2</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**
  - \( a' = \frac{(a - b)}{2} \)
  - \( b' = \frac{(a + b)}{2} \)
- **Along [1,1,1]**
  - \( a' = \frac{c}{3} \)
  - \( b' = -\frac{a + b}{2} \)
  - \( a' = \frac{2c}{3} \)
  - \( b' = -\frac{a + b}{2} \)
  - \( a' = \frac{c}{2} \)
  - \( b' = \frac{-(a + b)}{2} \)

#### Extended Symmetry

- **2d**
  - \( a' = \frac{a + b}{2} \)
  - \( b' = \frac{a - b}{2} \)
  - \( c' = \frac{c}{2} \)

- **2c**
  - \( a' = \frac{(a + b + c)}{3} \)
  - \( b' = -\frac{(a + b)}{3} \)
  - \( c' = \frac{c}{3} \)

- **2a**
  - \( a' = 0 \)
  - \( b' = 0 \)
  - \( c' = 0 \)

#### Symmetry of Planes

- **[001]**
  - \( a = b \)
  - \( c = 0 \)
- **[100]**
  - \( a = 0 \)
  - \( b = 0 \)
  - \( c = 0 \)
- **[111]**
  - \( a = b = c \)

#### Symmetry of Axes

- **[001]**
  - \( a = b \)
  - \( c = 0 \)
- **[100]**
  - \( a = 0 \)
  - \( b = 0 \)
  - \( c = 0 \)
- **[111]**
  - \( a = b = c \)
Origin at 4'32'

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad z \leq \min(x,1/2-x,y,1/2-y) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 0,1/2,0 & \quad 1/4,1/4,1/4 \\
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) \quad & 1 \\
& (1|0,0,0) \\
(2) \quad & 2 \quad 0,0,z \\
& (2|0,0,0) \\
(3) \quad & 2 \quad 0,y,0 \\
& (2|0,0,0) \\
(4) \quad & 2 \quad x,0,0 \\
& (2|0,0,0) \\
(5) \quad & 3^+ \quad x,x,x \\
& (3_{xyz}|0,0,0) \\
(6) \quad & 3^+ \quad x,x,x \\
& (3_{xyz}^{-1}|0,0,0) \\
(7) \quad & 3^+ \quad x,x,x \\
& (3_{xyz}^{-1}|0,0,0) \\
(8) \quad & 3^+ \quad x,x,x \\
& (3_{xyz}^{-1}|0,0,0) \\
(9) \quad & 3^- \quad x,x,x \\
& (3_{xyz}^{-1}|0,0,0) \\
(10) \quad & 3^- \quad x,x,x \\
& (3_{xyz}^{-1}|0,0,0) \\
(11) \quad & 3^- \quad x,x,x \\
& (3_{xyz}^{-1}|0,0,0) \\
(12) \quad & 3^- \quad x,x,x \\
& (3_{xyz}^{-1}|0,0,0) \\
\end{align*}
\]
Continued

(13) $2' \ x,x,0$
(20) $2' \ y,y,0$
(27) $2' \ x,x,0$
(34) $2' \ y,y,0$

For $(1/2,1/2,1/2)^{'} +$ set

(1) $t(1/2,1/2,1/2)^{'}$
(2) $2' (0,0,1/2)$
(3) $2' (0,1/2,0)$
(4) $2' (1/2,0,0)$

(5) $3^{+} (1/2,1/2,1/2) x,x,x$
(6) $3^{+} (1/6,-1/6,1/6) x+1/3,x+1/3,x$
(7) $3^{+} (-1/6,1/6,1/6) x+2/3,x-1/3,x$
(8) $3^{+} (1/6,1/6,-1/6) x+1/3,x+2/3,x$

(9) $3^{+} (1/2,1/2,1/2) x,x,x$
(10) $3^{+} (-1/6,1/6,1/6) x+1/3,x+1/3,x$
(11) $3^{+} (1/6,1/6,-1/6) x+2/3,x+1/3,x$
(12) $3^{+} (1/6,1/6,-1/6) x-1/3,x+2/3,x$

(13) $2 (1/2,1/2,0) x,x,1/4$
(14) $2 x,x+1/2,1/4$
(15) $4' (0,0,1/2) 1/2,0,z$
(16) $4^{+} (0,0,1/2) 0,1/2,z$

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2)'

48 $j$ 1

(1) $x,y,z \ [u,v,w]$ (2) $\bar{x},\bar{y},\bar{z} \ [\bar{u},\bar{v},\bar{w}]$ (3) $x,y,z \ [u,v,w]$ (4) $x,y,z \ [u,v,w]$
(5) $z,x,y \ [w,u,v]$ (6) $z,x,y \ [w,u,v]$ (7) $\bar{z},\bar{x},\bar{y} \ [\bar{w},\bar{u},\bar{v}]$ (8) $\bar{z},\bar{x},\bar{y} \ [\bar{w},\bar{u},\bar{v}]$
(9) $y,z,x \ [v,w,u]$ (10) $\bar{y},\bar{z},\bar{x} \ [\bar{v},\bar{w},\bar{u}]$ (11) $y,z,x \ [v,w,u]$ (12) $\bar{y},\bar{z},\bar{x} \ [\bar{v},\bar{w},\bar{u}]$
(13) $y,z,x \ [\bar{v},\bar{u},\bar{w}]$ (14) $y,z,x \ [v,u,w]$ (15) $y,z,x \ [v,u,w]$ (16) $\bar{y},\bar{z},\bar{x} \ [\bar{v},\bar{u},\bar{w}]$
(17) $x,z,y \ [u,w,v]$ (18) $x,z,y \ [u,w,v]$ (19) $x,z,y \ [u,w,v]$ (20) $x,z,y \ [u,w,v]$
(21) $z,y,x \ [w,v,u]$ (22) $z,y,x \ [w,v,u]$ (23) $z,y,x \ [w,v,u]$ (24) $\bar{z},\bar{y},\bar{x} \ [\bar{w},\bar{v},\bar{u}]$

211.5.1560 - 2 - 3510
Symmetry of Special Projections

Along [0,0,1] \( p_4 4m'm' \)
\[ a^* = \frac{a - b}{2}, \quad b^* = \frac{a + b}{2} \]
Origin at 1/2,0,z

Along [1,1,1] \( p3m11' \)
\[ a^* = \frac{2a - b - c}{3}, \quad b^* = \frac{-a + 2b - c}{3} \]
Origin at x,x,x

Along [1,1,0] \( p_2 2m'm' \)
\[ a^* = \frac{c}{2}, \quad b^* = \frac{-a + b}{2} \]
Origin at x,x,1/4

211.5.1560 - 3 - 3511
Origin on 3 \([111]\) at midpoint of three non-intersecting pairs of parallel screw axes \(4_3\) and \(2_1\).

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 3/4; \quad -1/2 \leq z \leq 1/4; \quad \max(-y,x-1/2) \leq y \leq \min(-y+1/2,2x-y,2y-x,y-2x+1/2)\]

Vertices

\((0,0,0)\), \((3/8,1/8,-1/8)\), \((1/2,1/2,0)\), \((1/4,3/4,-1/4)\), \((0,1/2,-1/2)\), \((1/4,1/4,1/4)\)

Symmetry Operations

1. \(1\)
2. \(2 \cdot (0,0,1/2)\) \(\quad 1/4,0,z\)
3. \(2 \cdot (0,1/2,0)\) \(\quad 0,y,1/4\)
4. \(2 \cdot (1/2,0,0)\) \(\quad x,1/4,0\)
5. \(3^+ \times,\times,\times\)
   \(\quad (3_{xyz}^{-1} \times,\times,\times)\)
6. \(3^+ \times+1/2,\times,\times\)
   \(\quad (3_{xyz}^{-1} \times,\times,\times)\)
7. \(3^+ \times+1/2,\times-1/2,\times\)
   \(\quad (3_{xyz}^{-1} \times,\times,\times)\)
8. \(3^+ \times,\times+1/2,\times\)
   \(\quad (3_{xyz}^{-1} \times,\times,\times)\)
9. \(3^- \times,\times,\times\)
   \(\quad (3_{xyz}^{-1} \times,\times,\times)\)
10. \(3^- (-1/3,1/3,1/3)\)
    \(\quad \times+1/6,\times+1/6,\times\)
11. \(3^- (1/3,1/3,-1/3)\)
    \(\quad \times+1/3,\times+1/3,\times\)
12. \(3^- (1/3,-1/3,1/3)\)
    \(\quad \times-1/6,\times+1/3,\times\)
Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 e 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12 d .2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 c .3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 b .32</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 a .32</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4g'm'</th>
<th>Along [1,1,1]</th>
<th>p3m'1</th>
<th>Along [1,1,0]</th>
<th>p2m'g'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = a</td>
<td>b* = b</td>
<td>a* = (2a - b - c)/3</td>
<td>b* = (-a + 2b - c)/3</td>
<td>a* = c</td>
<td>b* = -(a + b)/2</td>
</tr>
<tr>
<td>Origin at 1/4,1/2,z</td>
<td>Origin at x,x,x</td>
<td></td>
<td></td>
<td>Origin at x,x,x</td>
<td></td>
</tr>
</tbody>
</table>
Origin on 31' [111] at midpoint of three non-intersecting pairs of parallel screw axes 431' and 211'

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 3/4; -1/2 ≤ z ≤ 1/4; max (-y,x-1/2) ≤ y ≤ min(-y+1/2,2x-y,y-2x+1/2)

Vertices
0,0,0 3/8,1/8,-1/8 1/2,1/2,0 1/4,3/4,-1/4 0,1/2,-1/2 1/4,1/4,1/4

Symmetry Operations

For 1 + set

(1) 1
(1 | 0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z
(2 | 1/2,0,1/2)

(3) 2 (0,1/2,0) 0,y,1/4
(2 | 0,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2 | 1/2,1/2,0)

(5) 3' x,x,x
(3xyz | 0,0,0)

(6) 3* x+1/2,x,x
(3xyz' | 1/2,1/2,0)

(7) 3* x+1/2,x-1/2,x
(3xyz-1 | 1/2,0,1/2)

(8) 3* x,x+1/2,x
(3xyz-1 | 0,1/2,1/2)

(9) 3' x,x,x
(3xyz-1 | 0,0,0)

(10) 3* x+1/6,x+1/6,x
(3xyz | 0,1/2,1/2)

(11) 3* x+1/3,x+1/6,x
(3xyz | 1/2,1/2,0)

(12) 3* x-1/6,x+1/3,x
(3xyz | 1/2,0,1/2)

212.2.1562 - 1 - 3514
Continued 212.2.1562 P4₃ 321'

For 1' + set

1'  
(1) 1'  
(0,0,0)'  
(2) 2'  
(0,0,1/2)  
(1/2,0,1/2)'  
(3) 2'  
(0,1/2,0)  
(0,1/2,0)'  
(4) 2'  
(1/2,0,0)  
(1/2,0,1/2)'  

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 e 11'

1 + 1'

(1) x,y,z [0,0,0]  
(2) x+1/2,y,z+1/2 [0,0,0]  
(3) x,y+1/2,z+1/2 [0,0,0]  
(4) x+1/2,y+1/2,z [0,0,0]  

(5) z,x,y [0,0,0]  
(6) z+1/2,x+1/2,y [0,0,0]  
(7) z+1/2,x,y+1/2 [0,0,0]  
(8) z+1/2,y+1/2,z [0,0,0]  

(9) y,z,x [0,0,0]  
(10) y,z+1/2,x+1/2 [0,0,0]  
(11) y+1/2,z+1/2,x [0,0,0]  
(12) y+1/2,z,x+1/2 [0,0,0]  

(13) y+1/4,x+3/4,z+3/4 [0,0,0]  
(14) y+1/4,x+1/4,z+1/4 [0,0,0]  
(15) y+3/4,x+3/4,z+1/4 [0,0,0]  
(16) y+3/4,x+1/4,z+3/4 [0,0,0]  

(17) x+1/4,z+3/4,y+3/4 [0,0,0]  
(18) x+3/4,z+1/4,y+3/4 [0,0,0]  
(19) x+1/4,z+1/4,y+1/4 [0,0,0]  
(20) x+3/4,z+3/4,y+1/4 [0,0,0]  

(21) z+1/4,y+3/4,x+3/4 [0,0,0]  
(22) z+3/4,y+3/4,x+1/4 [0,0,0]  
(23) z+3/4,y+1/4,x+3/4 [0,0,0]  
(24) z+1/4,y+1/4,x+1/4 [0,0,0]  

212.2.1562 - 2 - 3515
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along</th>
<th>p4gm1'</th>
<th>p3m11'</th>
<th>p2mg1'</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[0,0,1]</td>
<td>[1,1,1]</td>
<td>[1,1,0]</td>
</tr>
<tr>
<td><strong>a</strong> = a</td>
<td><strong>b</strong> = b</td>
<td><strong>a</strong> = (2a - b - c)/3</td>
<td><strong>a</strong> = c</td>
</tr>
<tr>
<td><strong>b</strong> = b</td>
<td>Origin at 1/4,1/2,z</td>
<td><strong>b</strong> = (-a + 2b - c)/3</td>
<td><strong>b</strong> = -(-a + b)/2</td>
</tr>
<tr>
<td><strong>Origin at x,x,x</strong></td>
<td></td>
<td><strong>Origin at x,x</strong></td>
<td><strong>Origin at x,x+1/4,3/8</strong></td>
</tr>
</tbody>
</table>
Origin on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes $4_3'$ and $2_1$.

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 3/4; \quad -1/2 \leq z \leq 1/4; \quad \max(-y,x-1/2) \leq y \leq \min(-y+1/2,2x-y,2y-x,y-2x+1/2)
\]

Vertices

\[
0,0,0 \quad 3/8,1/8,-1/8 \quad 1/2,1/2,0 \quad 1/4,3/4,-1/4 \quad 0,1/2,-1/2 \quad 1/4,1/4,1/4
\]

Symmetry Operations

1. $1$
2. $2 (0,0,1/2) \quad 1/4,0,z$
   (2) $1/2,0,1/2$
3. $2 (0,1/2,0) \quad 0,y,1/4$
   (2) $0,1/2,1/2$
4. $2 (1/2,0,0) \quad x,1/4,0$
   (2) $1/2,1/2,0$
5. $3^+ \ x,x,x$
   (5) $3^+ x,x,0$
   (2) $1/2,1/2,0$
6. $3^+ \ x+1/2,x,\bar{x}$
   (3) $1/2,0,1/2$
7. $3^+ \ x+1/2,\bar{x}-1/2,\bar{x}$
   (3) $1/2,0,1/2$
8. $3^+ \ \bar{x},\bar{x}+1/2,\bar{x}$
   (3) $0,1/2,1/2$
9. $3^- \ x,x,x$
   (9) $3^- x,x,0$
   (2) $1/2,1/2,0$
10. $3^- x+1/6,x+1/6,x$
   (2) $1/2,1/2,0$
11. $3^- x+1/3,x+1/6,x$
   (2) $1/2,1/2,0$
12. $3^- (1/3,-1/3,1/3)$
   (2) $1/2,0,1/2$

212.3.1563 - 1 - 3517
Continued

212.3.1563  
P4$_3$ '32'

<table>
<thead>
<tr>
<th>Generators selected</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).</td>
</tr>
</tbody>
</table>

### Positions

- **Multiplicity**
- **Wyckoff letter**
- **Site Symmetry**

<table>
<thead>
<tr>
<th>(1) x,y,z [u,v,w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) x+1/2,y,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(3) x,y+1/2,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(4) x+1/2,y+1/2,z [u,v,w]</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
</tr>
<tr>
<td>(6) z+1/2,x+1/2,y [w,u,v]</td>
</tr>
<tr>
<td>(7) z+1/2,x,y+1/2 [w,u,v]</td>
</tr>
<tr>
<td>(8) z,x+1/2,y+1/2 [w,u,v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
</tr>
<tr>
<td>(10) y,z+1/2,x+1/2 [v,w,u]</td>
</tr>
<tr>
<td>(11) y+1/2,z+1/2,x [v,w,u]</td>
</tr>
<tr>
<td>(12) y+1/2,z,x+1/2 [v,w,u]</td>
</tr>
<tr>
<td>(13) y+1/4,x+3/4,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td>(14) y+1/4,x+1/4,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>(15) y+3/4,x+3/4,z+1/4 [v,u,w]</td>
</tr>
<tr>
<td>(16) y+3/4,x+1/4,z+3/4 [v,u,w]</td>
</tr>
<tr>
<td>(17) x+1/4,z+3/4,y+3/4 [u,v,w]</td>
</tr>
<tr>
<td>(18) x+3/4,z+1/4,y+3/4 [u,v,w]</td>
</tr>
<tr>
<td>(19) x+1/4,z+1/4,y+1/4 [w,u,v]</td>
</tr>
<tr>
<td>(20) x+3/4,z+3/4,y+1/4 [u,v,w]</td>
</tr>
<tr>
<td>(21) z+1/4,y+3/4,x+3/4 [w,u,v]</td>
</tr>
<tr>
<td>(22) z+3/4,y+1/4,x+3/4 [w,u,v]</td>
</tr>
<tr>
<td>(23) z+3/4,y+1/4,x+3/4 [w,v,u]</td>
</tr>
<tr>
<td>(24) z+1/4,y+1/4,x+1/4 [w,v,u]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 d .2' 1/8,y+1/4 [u,v,w] 3/8,y+3/4 [u,v,w] 7/8,y+1/4 [u,v,w] 5/8,y+1/2,y+3/4 [u,v,w]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8 c .3' x,x,x [u,u,u] x+1/2,x,x+1/2 [u,u,u] x+1/2,x+1/2 [u,u,u] x+1/2,x+1/2 [u,u,u]</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x+1/2,x+1/2 [u,u,u] x+1/2,x+1/2 [u,u,u] x+1/4,x+3/4,x+3/4 [u,u,u] x+1/4,x+3/4,x+1/4 [u,u,u]</td>
</tr>
<tr>
<td>x+3/4,x+3/4,x+1/4 [u,u,u] x+3/4,x+1/4,x+3/4 [u,u,u]</td>
</tr>
</tbody>
</table>

|-------------|

### Symmetry of Special Projections

- **Along [0,0,1]**  
P4'g'm
- **Along [1,1,1]**  
P3m1
- **Along [1,1,0]**  
P2'm'g

**a' = a**  
**b' = b**

**Origin at 1/4,1/2,z**

- **Along [0,0,1]**
  - **a' = 2a - b, c' = 3b**  
  - **Origin at x,x,x**

- **Along [1,1,1]**
  - **a' = (2a - b) / 3, b' = (b + 2c) / 3**  
  - **Origin at x,x,x**

- **Along [1,1,0]**
  - **a' = c, b' = -a + b / 2**  
  - **Origin at x,x,x+1/4,3/8**

212.3.1563 - 2 - 3518
Origin on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes 4₁ and 2₁

Asymmetric unit

\[-1/4 \leq x \leq 1/2; \quad 0 \leq y \leq 3/4; \quad 0 \leq z \leq 1/2; \quad x \leq y \leq x+1/2;\]

\[(y-x)/2 \leq z \leq \min(y,(-4x-2y+3)/2,(3-2x-2y)/4)\]

Vertices

0,0,0 1/2,1/2,0 1/4,3/4,1/4 -1/4,1/4,1/4 0,1/2,1/2 3/8,3/8,3/8

Symmetry Operations

(1) 1
(1) 0,0,0

(5) 3⁺ x,x,x
(3)xyz | 0,0,0

(6) 3⁺ x+1/2,x,x
(3)xyz⁻¹ | 1/2,1/2,0

(9) 3⁻ x,x,x
(3)xyz⁻¹ | 0,0,0

(10) 3⁻ (-1/3,1/3,1/3) x+1/6,x+1/6,x
(3)xyz⁻¹ | 0,1/2,1/2

(11) 3⁻ (1/3,1/3,-1/3) x+1/3,x+1/3,x
(3)xyz⁻¹ | 1/2,1/2,0

(12) 3⁻ (1/3,-1/3,1/3) x-1/6,x+1/3,x
(3)xyz⁻¹ | 1/2,0,1/2
Continued

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24 e 1

(1) x,y,z [u,v,w] (2) x+1/2,y,z+1/2 [u,v,w] (3) x,y+1/2,z+1/2 [u,v,w] (4) x+1/2,y+1/2,z [u,v,w]

(5) z,x,y [w,u,v] (6) z+1/2,x+1/2,y [w,u,v] (7) z+1/2,x,y+1/2 [w,u,v] (8) z,x+1/2,y+1/2 [w,u,v]

(9) y,z,x [v,w,u] (10) y,z+1/2,x+1/2 [v,w,u] (11) y+1/2,z+1/2,x [v,w,u] (12) y+1/2,z,x+1/2 [v,w,u]

(13) y+3/4,x+1/4,z+1/4 [v,u,w] (14) y+3/4,x+3/4,z+3/4 [v,u,w] (15) y+1/4,x+1/4,z+3/4 [v,u,w] (16) y+1/4,x+3/4,z+1/4 [v,u,w]

(17) x+3/4,z+1/4,y+1/4 [u,w,v] (18) x+1/4,z+3/4,y+1/4 [u,w,v] (19) x+3/4,z+3/4,y+3/4 [u,w,v] (20) x+1/4,z+1/4,y+3/4 [u,w,v]

(21) z+3/4,y+1/4,x+1/4 [w,v,u] (22) z+1/4,y+1/4,x+3/4 [w,v,u] (23) z+1/4,y+3/4,x+1/4 [w,v,u] (24) z+3/4,y+3/4,x+3/4 [w,v,u]

12 d .2 1/8,y+1/4,0 [v,v,0] 3/8,y+3/4,0 [v,v,0] 7/8,y+1/2,0 [v,v,0] 5/8,y+1/2,0 [v,v,0]

y+1/4,1/8,0 [v,v,0] y+3/4,3/8,0 [v,v,0] y+1/4,7/8,1/2 [v,v,0] y+3/4,5/8,1/2 [v,v,0]

y,y+1/4,1/8 [v,v,0] y,y+3/4,3/8 [v,v,0] y,y+1/4,7/8 [v,v,0] y,y+3/4,5/8 [v,v,0]

8 c .3 x,x,x [u,u,u] x+1/2,x,x+1/2 [u,u,u] x+1/2,x+1/2,x [u,u,u]

x+3/4,x,1/4 [u,u,u] x+3/4,x+1/4,x+1/4 [u,u,u] x+1/4,x+1/4,x+3/4 [u,u,u] x+1/4,x+3/4,x+1/4 [u,u,u]

4 b .32 7/8,7/8,7/8 [0,0,0] 5/8,7/8,3/8 [0,0,0] 1/8,3/8,5/8 [0,0,0] 3/8,5/8,1/8 [0,0,0]

4 a .32 3/8,3/8,3/8 [0,0,0] 1/8,5/8,7/8 [0,0,0] 5/8,7/8,1/8 [0,0,0] 7/8,1/8,5/8 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4g'm' a* = a b* = b

Origin at 1/4,0,z

Along [1,1,1] p3m'1 a* = (2a - b - c)/3 b* = (-a + 2b - c)/3

Origin at x,x,x

Along [1,1,0] p2m'q' a* = c b* = -(a + b)/2

Origin at x,x+1/4,1/8

213.1.1564 - 2 - 3520
Origin on 31' [111] at midpoint of three non-intersecting pairs of parallel screw axes 4,1' and 2,1'

Asymmetric unit

\[-\frac{1}{4} \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{3}{4}; \quad 0 \leq z \leq \frac{1}{2}; \quad x \leq y \leq x+\frac{1}{2};\]

\[(y-x)/2 \leq z \leq \min(y,(-4x-2y+3)/2,(3-2x-2y)/4)\]

Vertices

\[
\begin{align*}
0,0,0 & & 1/2,1/2,0 & & 1/4,3/4,1/4 & & -1/4,1/4,1/4 & & 0,1/2,1/2 & & 3/8,3/8,3/8
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & & \begin{pmatrix} 1 \end{pmatrix} \begin{pmatrix} 1 \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} & & \begin{pmatrix} 1 \end{pmatrix} \begin{pmatrix} 0,1/2 \end{pmatrix} \begin{pmatrix} 1/4,0,z \end{pmatrix} & & \begin{pmatrix} 3 \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} 0,y,1/4 \end{pmatrix} & & \begin{pmatrix} 4 \end{pmatrix} \begin{pmatrix} 1/2,0,0 \end{pmatrix} \begin{pmatrix} x,1/4,0 \end{pmatrix} \\
(2) & & \begin{pmatrix} 2 \end{pmatrix} \begin{pmatrix} 0,0,1/2 \end{pmatrix} \begin{pmatrix} 1/4,0,z \end{pmatrix} & & \begin{pmatrix} 1/2 \end{pmatrix} \begin{pmatrix} 2,0,1/2 \end{pmatrix} & & \begin{pmatrix} 3 \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} 0,y,1/4 \end{pmatrix} & & \begin{pmatrix} 2 \end{pmatrix} \begin{pmatrix} 1/2,1/2 \end{pmatrix} \begin{pmatrix} 1/2,1/2,0 \end{pmatrix} \\
(5) & & \begin{pmatrix} 3^+ \end{pmatrix} \begin{pmatrix} x,0,0 \end{pmatrix} \begin{pmatrix} x,x,x \end{pmatrix} & & \begin{pmatrix} 3^+ \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} x+1/2,x,x \end{pmatrix} & & \begin{pmatrix} 3^+ \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix} \begin{pmatrix} x+1/2,x,x \end{pmatrix} & & \begin{pmatrix} 3^+ \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} x+1/2,x,x \end{pmatrix} \\
& & \begin{pmatrix} 3_{x,y,z} \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} & & \begin{pmatrix} 3_{x,y,z} \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} 1/2,1/2,0 \end{pmatrix} & & \begin{pmatrix} 3_{x,y,z} \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix} \begin{pmatrix} x+1/2,x,x \end{pmatrix} & & \begin{pmatrix} 3_{x,y,z} \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} x+1/2,x,x \end{pmatrix} \\
(9) & & \begin{pmatrix} 3^- \end{pmatrix} \begin{pmatrix} x,0,0 \end{pmatrix} \begin{pmatrix} x,x,x \end{pmatrix} & & \begin{pmatrix} 3^- \end{pmatrix} \begin{pmatrix} -1/3,1/3,1/3 \end{pmatrix} \begin{pmatrix} x+1/6,x+1/6,x \end{pmatrix} & & \begin{pmatrix} 3^- \end{pmatrix} \begin{pmatrix} 1/3,-1/3,1/3 \end{pmatrix} \begin{pmatrix} x+1/3,x+1/3,x \end{pmatrix} & & \begin{pmatrix} 3^- \end{pmatrix} \begin{pmatrix} 1/3,-1/3,1/3 \end{pmatrix} \begin{pmatrix} x+1/3,x+1/3,x \end{pmatrix} \\
& & \begin{pmatrix} 3_{x,y,z}^{-1} \end{pmatrix} \begin{pmatrix} 0,0,0 \end{pmatrix} & & \begin{pmatrix} 3_{x,y,z}^{-1} \end{pmatrix} \begin{pmatrix} 0,1/2,0 \end{pmatrix} \begin{pmatrix} 1/2,1/2,0 \end{pmatrix} & & \begin{pmatrix} 3_{x,y,z}^{-1} \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix} \begin{pmatrix} x+1/3,x+1/3,x \end{pmatrix} & & \begin{pmatrix} 3_{x,y,z}^{-1} \end{pmatrix} \begin{pmatrix} 1/2,0,1/2 \end{pmatrix} \begin{pmatrix} x+1/3,x+1/3,x \end{pmatrix}
\end{align*}
\]
Continued

Coordinates

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.</td>
<td>Coordinates</td>
</tr>
</tbody>
</table>

213.2.1565 - 2 - 3522
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Origin at x,x,x</th>
<th>Along [1,0,0]</th>
<th>p4gm1'</th>
<th>a* = a  b* = b</th>
</tr>
</thead>
</table>

| Origin at x,x+1/4,0 | Along [1,1,1] | p3m11' | a* = (2a - b - c)/3  b* = (-a + 2b - c)/3 |

| Origin at x,x+1/4,1/8 | Along [1,1,0] | p2mg1' | a* = c  b* = (-a + b)/2 |

| Origin at 1/4,0,z | Along [0,0,1] | p4gm1' | a* = a  b* = b |

| Origin at x,x,x | Along [1,0,0] | p4gm1' | a* = a  b* = b |

| Origin at x,x+1/4,0 | Along [1,1,1] | p3m11' | a* = (2a - b - c)/3  b* = (-a + 2b - c)/3 |

| Origin at x,x+1/4,1/8 | Along [1,1,0] | p2mg1' | a* = c  b* = (-a + b)/2 |

| Origin at 1/4,0,z | Along [0,0,1] | p4gm1' | a* = a  b* = b |
Origin on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes 4' and 2₁.

Asymmetric unit

\[-1/4 \leq x \leq 1/2; \quad 0 \leq y \leq 3/4; \quad 0 \leq z \leq 1/2; \quad x \leq y \leq x+1/2;\]

\[(y-x)/2 \leq z \leq \min(y,(-4x-2y+3)/2,(3-2x-2y)/4)\]

Vertices

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1/2,1/2,0</th>
<th>1/4,3/4,1/4</th>
<th>-1/4,1/4,1/4</th>
<th>0,1/2,1/2</th>
<th>3/8,3/8,3/8</th>
</tr>
</thead>
</table>

Symmetry Operations

(1) 1
(2) 2 (0,0,1/2) 1/4,0,z
(2₁ | 1/2,0,1/2)
(3) 2 (0,1/2,0) 0,y,1/4
(2₁ | 0,1/2,1/2)
(4) 2 (1/2,0,0) x,1/4,0
(2₁ | 1/2,1/2,0)
(5) 3⁺ x,x,x
(3xyz | 0,0,0)
(6) 3⁺ x+1/2,x,x
(3xyz⁻¹ | 1/2,1,2,0)
(7) 3⁺ x+1/2,x,x-1/2,x
(3xyz⁻¹ | 1/2,0,1/2)
(8) 3⁺ x⁺1/2,x
(3xyz⁻¹ | 0,1/2,1/2)
(9) 3⁻ x,x,x
(3xyz⁻¹ | 0,0,0)
(10) 3⁻ (-1/3,1/3,1/3)
(3xyz⁻¹ | 1/2,1/2,0)
(11) 3⁻ (1/3,1/3,-1/3)
(3xyz⁻¹ | 1/2,1/2,0)
(12) 3⁻ (1/3,-1/3,1/3)
(3xyz⁻¹ | 1/2,0,1/2)
Continued 213.3.1566  P4₁ 32'

(13) 2' (1/2,1/2,0)  x,x-1/4,1/8  
(2ₚ) 3/4,1/4,1/4')

(14) 2' x,x+3/4,3/8
(2ₚ) 3/4,3/4,3/4')

(15) 4' (0,0,3/4) 1/4,0,z  
(4₋₁) 1/4,1/4,3/4')

(16) 4' (0,0,1/4) -1/4,1/2,z
(4₋₁) 1/4,1/4,3/4')

(17) 4' (3/4,0,0)  x,1/4,0
(4₋₁) 3/4,1/4,1/4')

(18) 2' (0,1/2,1/2) 1/8,y+1/4,y
(2ₚ) 1/4,3/4,3/4')

(19) 2' 3/8,y+3/4,y
(2ₚ) 3/4,3/4,3/4')

(20) 4' (1/4,0,0) x,-1/4,1/2
(4₋₁) 1/4,1/4,3/4')

(21) 4' (0,1/4,0) 1/2,y,-1/4
(4₋₁) 3/4,1/4,1/4')

(22) 2' (1/2,0,1/2)  x-1/4,1/8,x
(2ₚ) 1/4,1/4,3/4')

(23) 4' (0,3/4,0) 0,y,1/4
(4₋₁) 1/4,1/4,3/4')

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

24.e 1

(1) x,y,z [u,v,w]  
(2) x+1/2,y,z+1/2 [u,v,w]  
(3) x,y+1/2,z+1/2 [u,v,w]  
(4) x+1/2,y+1/2,z [u,v,w]  

(5) z,x,y [w,u,v]  
(6) z+1/2,x,y+1/2 [w,u,v]  
(7) z+1/2,x,y+1/2 [w,u,v]  
(8) z,x+1/2,y+1/2 [w,u,v]  

(9) y,z,x [v,w,u]  
(10) y,z+1/2,x+1/2 [v,w,u]  
(11) y+1/2,z,x+1/2 [v,w,u]  
(12) y+1/2,z,x+1/2 [v,w,u]  

(13) y+3/4,x+1/4,z+1/4 [v,u,w]  
(14) y+3/4,x+3/4,z+3/4 [v,u,w]  
(15) y+1/4,x+1/4,z+3/4 [v,u,w]  
(16) y+1/4,x+3/4,z+1/4 [v,u,w]  

(17) x+3/4,z+1/4,y+1/4 [u,v,w]  
(18) x+1/4,z+3/4,y+1/4 [u,v,w]  
(19) x+3/4,z+3/4,y+3/4 [u,v,w]  
(20) x+1/4,z+1/4,y+3/4 [u,v,w]  

(21) z+3/4,y+1/4,x+1/4 [w,v,u]  
(22) z+1/4,y+1/4,x+1/4 [w,v,u]  
(23) z+1/4,y+3/4,x+1/4 [w,v,u]  
(24) z+3/4,y+3/4,x+1/4 [w,v,u]  

12.d .2' 1/8,y,y+1/4 [u,v,v]  
3/8,y,y+3/4 [u,v,v]  
7/8,y+1/2,y+1/4 [u,v,v]  
5/8,y+1/2,y+3/4 [u,v,v]  

y+1/4,1/8,y [v,u,v]  
y+3/4,3/8,y [u,v,v]  
y+1/4,7/8,y+1/2 [v,u,v]  
y+3/4,5/8,y+1/2 [v,u,v]  

y,y+1/4,1/8 [v,u,v]  
y,y+3/4,3/8 [v,u,v]  
y+1/2,y+1/4,7/8 [v,u,v]  
y+1/2,y+3/4,5/8 [v,u,v]  

8.c .3. x,x,x [u,u,u]  
3/8,y,y+3/4 [u,v,v]  
7/8,y+1/2,y+1/4 [u,v,v]  
5/8,y+1/2,y+3/4 [u,v,v]  

x+1/2,x+1/2 [u,u,u]  
x+3/4,x+1/4,x+1/4 [u,u,u]  
x+1/4,x+1/4,x+3/4 [u,u,u]  

4.b .32' 7/8,7/8,7/8 [u,u,u]  
5/8,1/8,3/8 [u,u,u]  
1/8,3/8,5/8 [u,u,u]  
3/8,5/8,1/8 [u,u,u]  

4.a .32' 3/8,3/8,3/8 [u,u,u]  
1/8,5/8,7/8 [u,u,u]  
5/8,7/8,1/8 [u,u,u]  
7/8,1/8,5/8 [u,u,u]  

Symmetry of Special Projections

Along [0,0,1]  p4'g'm  
Along [1,1,1]  p3m1  
Along [1,1,0]  p2'mg'

a* = a  b* = b
Origin at 1/4,0,z

a* = (2a - b - c)/3  b* = (-a + 2b - c)/3
Origin at x,x,x

a* = c  b* = (-a + b)/2
Origin at x,x+1/4,1/8
Origin on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes 41 and 43 and of three non-intersection pairs of parallel 2 axes.

Asymmetric unit

\[-\frac{3}{8} < x < \frac{1}{8}; \quad -\frac{1}{8} < y < \frac{1}{8}; \quad \frac{1}{8} < z < \frac{3}{8}; \quad \max(x, y, y - x - \frac{1}{8}) < z < y + \frac{1}{4}\]

Vertices

\[
\begin{align*}
1/8,1/8,1/8 & \quad 1/8,1/8,3/8 & \quad 1/8,-1/8,1/8 & \quad -1/8,1/8,1/8 & \quad -1/8,-1/8,-1/8 & \quad -3/8,1/8,3/8 & \quad -3/8,-1/8,1/8 \\
\end{align*}
\]

Symmetry Operations

For (0,0,0) + set

\[
\begin{align*}
(1) & \quad 1 & \quad (2) & \quad (0,0,1/2) & \quad 1/4,0,z & \quad (3) & \quad (0,1/2,0) & \quad 0,y,1/4 & \quad (4) & \quad (1/2,0,0) & \quad x,1/4,0 \\
& \quad (1|0,0,0) & \quad (2_z|1/2,0,1/2) & \quad (2_y|0,1/2,1/2) & \quad (2_x|1/2,1/2,0) & \\
(5) & \quad 3^+ x,x,x & \quad (6) & \quad 3^- x+1/2,x,x & \quad (7) & \quad 3^+ x+1/2,x-1/2,x & \quad (8) & \quad 3^- x,x+1/2,x & \\
& \quad (3_{xyz}|0,0,0) & \quad (3_{xyz}^{-1}|1/2,1/2,0) & \quad (3_{xyz}^{-1}|1/2,0,1/2) & \quad (3_{xyz}^{-1}|1,1/2,1/2) & \\
(9) & \quad 3^+ x,x,x & \quad (10) & \quad 3^- (-1/3,1/3,1/3) x+1/6,x+1/6,x & \quad (11) & \quad 3^+ (1/3,1/3,-1/3) x+1/3,x+1/3,x & \quad (12) & \quad 3^- (1/3,-1/3,1/3) x-1/6,x+1/3,x & \\
& \quad (3_{xyz}^{-1}|0,0,0) & \quad (3_{xyz}|0,1/2,1/2) & \quad (3_{xyz}^{-1}|1/2,1/2,0) & \quad (3_{xyz}^{-1}|2/2,0,1/2) & \\
\end{align*}
\]
Continued

(13) 2 (1/2,1/2,0) x,x-1/4,1/8
(2yz) 3/4,1/4,1/4

(14) 2 x,\(x+3/4,3/8\)
(2yz) 3/4,3/4,3/4

(15) 4\(\frac{1}{4}\),0,3/4) 1/4,0,z
(4z) 1/4,1/4,3/4

(16) 4\(\frac{1}{4}\),0,1/4) -1/4,1/2,z
(4z) 1/4,3/4,1/4

(17) 4\(\frac{1}{4}\),3/4,0) x,1/4,0
(4z) 3/4,1/4,1/4

(18) 2 (0,1/2,1/2) 1/8,y+1/4,y
(2yz) 1/4,3/4,1/4

(19) 2 3/8,y+3/4,y
(2yz) 3/4,3/4,3/4

(20) 4\(\frac{1}{4}\),0,0) x,-1/4,1/2
(4z) 1/4,1/4,3/4

(21) 4\(\frac{1}{4}\),0,1/4) 1/2,y,-1/4
(4z) 3/4,1/4,1/4

(22) 2 (1/2,0,1/2) x-1/4,1/8,x
(2yz) 1/4,1/4,3/4

(23) 4\(\frac{1}{4}\),0,3/4) 0,y,1/4
(4z) 1/4,3/4,1/4

(24) 2 x+3/4,3/8,x
(2yz) 3/4,3/4,3/4

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(2) 2 0,1/4,z
(3) 2 1/4,y,0
(4) 2 x,0,1/4
(2z) 0,1/2,0

(5) 3\(\frac{1}{2}\) (1/2,1/2,1/2) x,x,x
(6) 3\(\frac{1}{2}\) (1/6,-1/6,1/6)
(7) 3\(\frac{1}{2}\) -1/6,1/6,1/6
(8) 3\(\frac{1}{2}\) (1/6,1/6,1/6)

(3) x,y,z [u,v,w] (1/2,1/2,1/2)
(z) x+1/6,x+1/6,x

(9) 3\(\frac{1}{2}\) (1/2,1/2,1/2) x,x,x
(10) 3\(\frac{1}{2}\) (1/6,-1/6,1/6)
(11) 3\(\frac{1}{2}\) -1/6,-1/6,1/6
(12) 3\(\frac{1}{2}\) (1/6,1/6,1/6)

(3) x,y,z [u,v,w] (1/2,1/2,1/2)
(z) x+1/6,x+1/6,x

(13) 2 (1/2,1/2,0) x,x+1/4,3/8
(2yz) 1/4,3/4,3/4

(14) 2 x,\(x+1/4,1/8\)
(2yz) 1/4,1/4,1/4

(15) 4\(\frac{1}{4}\),0,0) 3/4,0,z
(4z) 3/4,3/4,3/4

(16) 4\(\frac{1}{4}\),0,3/4) 1/4,1/2,z
(4z) 3/4,1/4,3/4

(17) 4\(\frac{1}{4}\),1/4,0) x,3/4,0
(4z) 1/4,3/4,3/4

(18) 2 (0,1/2,1/2) 3/8,y-1/4,y
(2yz) 3/4,1/4,3/4

(19) 2 1/8,y-1/4,y
(2yz) 1/4,1/4,1/4

(20) 4\(\frac{1}{4}\),0,0) x,1/4,1/2
(4z) 3/4,3/4,1/4

(21) 4\(\frac{1}{4}\),0,3/4) 1/2,y,1/4
(4z) 1/4,3/4,3/4

(22) 2 (1/2,0,1/2) x+1/4,3/8,x
(2yz) 3/4,3/4,3/4

(23) 4\(\frac{1}{4}\),0,1/4) 0,y,3/4
(4z) 3/4,1/4,3/4

(24) 2 x+1/4,1/8,x
(2yz) 1/4,1/4,1/4

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) + (1/2,1/2,1/2) + 48 i 1

(1) x,y,z [u,v,w] (2) \(\bar{x}+1/2,\bar{y},z+1/2\) [\(\bar{u},\bar{v},\bar{w}\)] (3) x,y+1/2,z+1/2 [u,v,w] (4) x+1/2,\(\bar{y}+1/2,\bar{z}\) [u,\(\bar{v},\bar{w}\)]

(5) z,x,y [w,u,v] (6) z+1/2,x+1/2,\(\bar{y}\) [w,\(\bar{u},\bar{v}\)] (7) \(\bar{z}+1/2,\bar{x},y+1/2\) [w,u,v] (8) \(\bar{z},x+1/2,\bar{y}+1/2\) [w,u,v]

(9) y,z,x [v,w,u] (10) \(\bar{y},z+1/2,\bar{x}+1/2\) [v,\(\bar{w},\bar{u}\)] (11) y+1/2,\(\bar{z}+1/2,\bar{x}\) [v,w,u] (12) \(\bar{y}+1/2,\bar{z},x+1/2\) [v,\(\bar{w},\bar{u}\)]

(13) y+3/4,x+1/4,\(\bar{z}+1/4\) [v,u,w] (14) \(\bar{y}+3/4,\bar{x}+3/4,\bar{z}+3/4\) [\(\bar{v},\bar{u},\bar{w}\)] (15) y+1/4,\(\bar{x}+1/4,\bar{z}+3/4\) [v,u,w] (16) \(\bar{y}+1/4,\bar{x}+3/4,\bar{z}+1/4\) [v,u,w]

(17) x+3/4,z+1/4,\(y+1/4\) [u,w,v] (18) \(\bar{x}+1/4,\bar{z}+3/4,\bar{y}+1/4\) [u,w,v] (19) x+3/4,z+3/4,y+3/4 [u,\(\bar{w},\bar{v}\)] (20) x+1/4,z+1/4,y+3/4 [u,w,v]

(21) z+3/4,y+1/4,x+1/4 [w,v,\(\bar{u}\)] (22) z+1/4,\(y+1/4,x+3/4\) [w,v,u] (23) \(\bar{z}+1/4,y+3/4,x+1/4\) [w,v,u] (24) \(\bar{z}+3/4,\bar{y}+3/4,\bar{x}+3/4\) [v,\(\bar{w},\bar{u}\)]
| 24 | h | 1/8,y+1/4 [0,v,v] | 3/8,y+3/4 [0,v,v] | 7/8,y+1/2,y+1/4 [v,v,0] | 5/8,y+1/2,y+3/4 [0,v,v] |
| 24 | g | 1/8,y+1/4 [0,v,v] | y+3/4,3/8,y [v,0,v] | y+1/4,7/8,y+1/2 [v,0,v] | y+3/4,5/8,y+1/2 [v,0,v] |
| 24 | f | x,0,1/4 [u,0,0] | x+1/2,0,3/4 [u,0,0] | 1/4,x,0 [0,u,0] | 3/4,x+1/2,0 [0,u,0] |
| 16 | e | x,x,x [u,u,u] | x+1/2,x+1/2 [u,u,u] | x,x+1/2,x+1/2 [u,u,u] | x+3/4,x+1/4,x+1/4 [u,u,u] |
| 12 | d | 5/8,0,1/4 [0,0,0] | 7/8,0,3/4 [0,0,0] | 1/4,5/8,0 [0,0,0] | 3/4,7/8,0 [0,0,0] |
| 12 | c | 1/8,0,1/4 [0,0,0] | 3/8,0,3/4 [0,0,0] | 1/4,1/8,0 [0,0,0] | 3/4,3/8,0 [0,0,0] |
| 8  | b | 7/8,7/8,7/8 [0,0,0] | 5/8,1/8,3/8 [0,0,0] | 1/8,3/8,5/8 [0,0,0] | 3/8,5/8,1/8 [0,0,0] |
| 8  | a | 1/8,1/8,1/8 [0,0,0] | 3/8,7/8,5/8 [0,0,0] | 7/8,5/8,3/8 [0,0,0] | 5/8,3/8,7/8 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'

\[ a^* = (a - b)/2 \quad b^* = (a + b)/2 \]

Origin at 1/4,0,z

Along [1,1,1] p3m'1

\[ a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \quad c^* = c/2 \]

Origin at x,x,x

Along [1,1,0] p2m'm'

\[ a^* = -a + b/2 \quad b^* = c/2 \]

Origin at x,x+1/4,1/8

---

214.1.1567 - 3 - 3528
**Origin** on $31^1[111]$ at midpoint of three non-intersecting pairs of parallel screw axes $4,1^1$ and $4,1^1$ and of three non-intersection pairs of parallel 2 axes.

**Asymmetric unit**

$$-3/8 < x < 1/8; \quad -1/8 \leq y \leq 1/8; \quad 1/8 \leq z \leq 3/8; \quad \max(x,y,y - x - 1/8) \leq z \leq y+1/4$$

**Vertices**

$$1/8,1/8,1/8 \quad 1/8,1/8,3/8 \quad 1/8,-1/8,1/8 \quad -1/8,1/8,1/8 \quad -1/8,-1/8,-1/8 \quad -3/8,1/8,3/8 \quad -3/8,-1/8,1/8$$

**Symmetry Operations**

For $(0,0,0) +$ set

<table>
<thead>
<tr>
<th>Operation</th>
<th>Description</th>
<th>Matrix</th>
<th>Translation</th>
<th>Identity</th>
<th>$(1/2,0,0)$</th>
<th>$(1/2,1,2,0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1)$</td>
<td>$1$</td>
<td></td>
<td></td>
<td>$(1)$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td>$(2)$</td>
<td>$2(0,0,1/2)$</td>
<td>$1/4,0,z$</td>
<td>$(2)$</td>
<td>$1/2,0,1/2$</td>
<td>$0,1/2,0$</td>
<td>$1/2,1/2,0$</td>
</tr>
<tr>
<td>$(3)$</td>
<td>$2(0,1/2,0)$</td>
<td>$0,y,1/4$</td>
<td>$(3)$</td>
<td>$0,1/2,1/2$</td>
<td>$1/2,1/2,0$</td>
<td>$0,1/2,0$</td>
</tr>
<tr>
<td>$(4)$</td>
<td>$2(1/2,0,0)$</td>
<td>$x,1/4,0$</td>
<td>$(4)$</td>
<td>$1/2,1/2,0$</td>
<td>$0,1/2,0$</td>
<td>$1/2,0,0$</td>
</tr>
<tr>
<td>$(5)$</td>
<td>$3^+ x,x,x$</td>
<td></td>
<td></td>
<td>$(5)$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td>$(6)$</td>
<td>$3^+ x+1/2,x,x$</td>
<td></td>
<td></td>
<td>$(6)$</td>
<td>$1/2,1/2,0$</td>
<td>$1/2,1/2,0$</td>
</tr>
<tr>
<td>$(7)$</td>
<td>$3^+ x+1/2,x-1/2,x$</td>
<td></td>
<td></td>
<td>$(7)$</td>
<td>$0,1/2,1/2$</td>
<td>$0,1/2,0$</td>
</tr>
<tr>
<td>$(8)$</td>
<td>$3^- x,x+1/2,x$</td>
<td></td>
<td></td>
<td>$(8)$</td>
<td>$1/2,0,1/2$</td>
<td>$1/2,0,1/2$</td>
</tr>
<tr>
<td>$(9)$</td>
<td>$3^- x,x,x$</td>
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<td>$(9)$</td>
<td>$0,0,0$</td>
<td>$0,0,0$</td>
</tr>
<tr>
<td>$(10)$</td>
<td>$3^- x-1/3,1/3,1/3$</td>
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<td></td>
<td>$(10)$</td>
<td>$0,1/2,1/2$</td>
<td>$0,1/2,1/2$</td>
</tr>
<tr>
<td>$(11)$</td>
<td>$3^- x+1/3,1/3,-1/3$</td>
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<td></td>
<td>$(11)$</td>
<td>$1/2,1/2,0$</td>
<td>$1/2,1/2,0$</td>
</tr>
<tr>
<td>$(12)$</td>
<td>$3^- x-1/6,x+1/3,x$</td>
<td></td>
<td></td>
<td>$(12)$</td>
<td>$1/2,0,1/2$</td>
<td>$1/2,0,1/2$</td>
</tr>
</tbody>
</table>

**Diagram**

214.2.1568 - 1 - 3529
Continued 214.2.1568  I4, 321'

For (1/2,1/2,1/2) + set

(1) t' (1/2,1/2,1/2) (2) 2' 0,1/4, z (3) 2' 1/4, y, 0 (4) 2' x, 0,1/4
(1 1/2,1/2,1/2) (2') 0,1/2, 0' (2') 1/2,0,0' (2') 0,0,1/2'

(5) 3' - (1/2,1/2,1/2) x,x,x (6) 3' (1/6,-1/6,1/6) x-1/6,x+1/3,x (7) 3' - (1/6,1/6,1/6) x+1/6,x+1/6,x
(3xyz 1/2,1/2,1/2)' (3xyz -1/2,0,1/2)' (3xyz 1/2,0,0)'

(9) 3' (1/2,1/2,1/2) x,x,x (10) 3' (1/6,-1/6,-1/6) x+1/6,x+1/6,x (11) 3' (1/6,1/6,-1/6)
(3xyz -1/2,1/2,1/2)' (3xyz 0,1/2,0)' (3xyz 1/2,0,0)'

(13) 2' (1/2,1/2,0) x,x+1/4,3/8 (14) 2' x,x+1/4,1/8 (15) 4' (0,0,1/4) 3/4,0,z
(2xy 1/4,3/4,3/4)' (2xy 1/4,1/4,1/4)' (4z -1 3/4,3/4,1/4)'

(17) 4' (1/4,0,0) x,3,4,0 (18) 2' (0,1/2,1/2) 3/8,y-1/4,y (19) 2' (0,1/4,0)
(4z -1 1/4,3,4,3/4)' (2yz 3/4,1/4,1/4)' (4z 1/4,1/4,1/4)'

(21) 4' (0,3/4,0) 1/2,y,1/4 (22) 2' (1/2,0,1/2) x+1/4,3/8,x (23) 4' (0,1/4,0) 0,y,3/4
(4y 1/4,3,4,3/4)' (2xy 3/4,3,4,3/4)'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

    (0,0,0) +      (1/2,1/2,1/2) +
    (0,0,0)' +     (1/2,1/2,1/2)' +

48 i 11'

(1) x,y,z [0,0,0] (2) x+1/2,y,z+1/2 [0,0,0] (3) x,y+1/2,z+1/2 [0,0,0] (4) x+1/2,y+1/2,z [0,0,0]
(5) z,x,y [0,0,0] (6) z+1/2,x+1/2,y [0,0,0] (7) z+1/2,x,y+1/2 [0,0,0] (8) z,x+1/2,y+1/2 [0,0,0]
(9) y,z,x [0,0,0] (10) y,z+1/2,x+1/2 [0,0,0] (11) y+1/2,z+1/2,x [0,0,0] (12) y+1/2,z,x+1/2 [0,0,0]
(13) y+3/4,x+1/4,z+1/4 [0,0,0] (14) y+3/4,x+3/4,z+3/4 [0,0,0] (15) y+1/4,x+1/4,z+3/4 [0,0,0] (16) y+1/4,x+3/4,z+1/4 [0,0,0]
(17) x+3/4,z+1/4,y+1/4 [0,0,0] (18) x+1/4,z+3/4,y+1/4 [0,0,0] (19) x+3/4,z+3/4,y+3/4 [0,0,0] (20) x+1/4,z+1/4,y+3/4 [0,0,0]
(21) z+3/4,y+1/4,x+1/4 [0,0,0] (22) z+1/4,y+1/4,x+3/4 [0,0,0] (23) z+1/4,y+3/4,x+1/4 [0,0,0] (24) z+3/4,y+3/4,x+3/4 [0,0,0]

24 h .21' 1/8,y,x+1/4 [0,0,0] 3/8,y,x+3/4 [0,0,0] 7/8,y+1/2,y+1/4 [0,0,0] 5/8,y+1/2,y+3/4 [0,0,0]
     y+1/4,1/8,y [0,0,0] y+3/4,3/8,y [0,0,0] y+1/4,7/8,y+1/2 [0,0,0] y+3/4,5/8,y+1/2 [0,0,0]
     y,y+1/4,1/8 [0,0,0] y,y+3/4,3/8 [0,0,0] y+1/2,y+1/4,7/8 [0,0,0] y+1/2,y+3/4,5/8 [0,0,0]
24 g .21' 1/8, y + 1/4 [0, 0, 0] 3/8, y, y + 3/4 [0, 0, 0] 7/8, y + 1/2, y + 1/4 [0, 0, 0] 5/8, y + 1/2, y + 1/4 [0, 0, 0] y + 1/4, 1/8, y [0, 0, 0] y + 3/4, 3/8, y [0, 0, 0] y + 1/4, 1/8, y [0, 0, 0] y + 3/4, 3/8, y [0, 0, 0] y + 1/2, y + 1/4, 1/8 [0, 0, 0] y + 3/4, 3/8, y + 1/2 [0, 0, 0] 24 f 2..1' x, 0, 1/4 [0, 0, 0] x + 1/2, 0, 3/4 [0, 0, 0] 1/4, x, 0 [0, 0, 0] 3/4, x + 1/2, 0 [0, 0, 0] 0, 1/4, x [0, 0, 0] 0, 3/4, x + 1/2 [0, 0, 0] 3/4, x + 1/4, 0 [0, 0, 0] 3/4, x + 3/4, 1/2 [0, 0, 0] x + 3/4, 1/2, 1/4 [0, 0, 0] x + 1/4, 0, 1/4 [0, 0, 0] 0, 1/4, x + 1/4 [0, 0, 0] 1/2, 1/4, x + 3/4 [0, 0, 0] 16 e .3.1' x, x, x [0, 0, 0] x + 1/2, x, x + 1/2 [0, 0, 0] x + 3/4, x + 1/4, x + 1/4 [0, 0, 0] x + 3/4, x + 3/4, x + 3/4 [0, 0, 0] x + 1/4, x + 1/4, x + 3/4 [0, 0, 0] x + 1/4, x + 3/4, x + 1/4 [0, 0, 0] 12 d 2.221' 5/8, 0, 1/4 [0, 0, 0] 7/8, 0, 3/4 [0, 0, 0] 1/4, 5/8, 0 [0, 0, 0] 3/4, 7/8, 0 [0, 0, 0] 0, 1/4, 5/8 [0, 0, 0] 0, 3/4, 7/8 [0, 0, 0] 12 c 2.221' 1/8, 0, 1/4 [0, 0, 0] 3/8, 0, 3/4 [0, 0, 0] 1/4, 1/8, 0 [0, 0, 0] 3/4, 3/8, 0 [0, 0, 0] 0, 1/4, 1/8 [0, 0, 0] 0, 3/4, 3/8 [0, 0, 0] 8 b .321' 7/8, 7/8, 7/8 [0, 0, 0] 5/8, 1/8, 3/8 [0, 0, 0] 1/8, 3/8, 5/8 [0, 0, 0] 3/8, 5/8, 1/8 [0, 0, 0] 8 a .321' 1/8, 1/8, 1/8 [0, 0, 0] 3/8, 7/8, 5/8 [0, 0, 0] 7/8, 5/8, 3/8 [0, 0, 0] 5/8, 3/8, 7/8 [0, 0, 0] 214.2.1568

Symmetry of Special Projections

Along [0, 0, 1] p4mm1' 
\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]
Origin at 1/4, 0, z

Along [1, 1, 1] p3m11' 
\[ \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \quad \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3 \]
Origin at x, x, x

Along [1, 1, 0] p2mm1' 
\[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \]
Origin at x, x + 1/4, 1/8
Origin on [111] at midpoint of three non-intersecting pairs of parallel screw axes $4_1'$ and $4_3'$ and of three non-intersection pairs of parallel 2 axes.

Asymmetric unit

$$\begin{align*}
-3/8 \leq x &\leq 1/8; \\
-1/8 \leq y &\leq 1/8; \\
1/8 \leq z &\leq 3/8; \\
\max(x,y,y-x-1/8) &\leq z \leq y+1/4
\end{align*}$$

Vertices

$$\begin{align*}
1/8,1/8,1/8 & \\
1/8,1/8,3/8 & \\
1/8,-1/8,1/8 & \\
-1/8,1/8,1/8 & \\
-1/8,-1/8,-1/8 & \\
-3/8,1/8,3/8 & \\
-3/8,-1/8,1/8 &
\end{align*}$$

Symmetry Operations

For $(0,0,0)$ + set

$$\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(2) & \quad 2 \quad (0,0,1/2) \\
(2) & \quad 1/4,0,z \\
(2_1) & \quad 1/2,0,1/2 \\
(2_2) & \quad 0,1/2,1/2 \\
(3) & \quad 2 \quad (0,1/2,0) \\
(3) & \quad 0,y,1/4 \\
(3_1) & \quad 0,1/2,1/2 \\
(3_2) & \quad 1/2,1/2,0 \\
(4) & \quad 2 \quad (1/2,0,0) \\
(4) & \quad x,1/4,0 \\
(4_1) & \quad 1/2,1/2,0 \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz} | 0,0,0) \\
(6) & \quad 3^+ \quad x+1/2,x,x \\
(6) & \quad (3_{xyz}^{-1} | 1/2,1/2,0) \\
(7) & \quad 3^+ \quad x+1/2,x-1/2,x \\
(7) & \quad (3_{xyz}^{-1} | 1/2,0,1/2) \\
(8) & \quad 3^+ \quad x,x+1/2,x \\
(8) & \quad (3_{xyz}^{-1} | 0,1/2,1/2) \\
(9) & \quad 3^- \quad x,x,x \\
(9) & \quad (3_{xyz}^{-1} | 0,0,0) \\
(10) & \quad 3^- \quad (-1/3,1/3,1/3) \\
(10) & \quad x+1/6,x+1/6,x \\
(10) & \quad (3_{xyz} | 0,1/2,1/2) \\
(11) & \quad 3^- \quad (1/3,1/3,-1/3) \\
(11) & \quad x+1/3,x+1/3,x \\
(11) & \quad (3_{xyz} | 1/2,1/2,0) \\
(12) & \quad 3^- \quad (1/3,-1/3,1/3) \\
(12) & \quad x-1/6,x+1/3,x \\
(12) & \quad (3_{xyz}^{-1} | 1/2,0,1/2) \\
\end{align*}$$
(13) 2' (1/2,1/2,0) x,x-1/4,1/8
(2y) 3/4,1/4,1/4)

(14) 2' x,x+3/4,3/8
(2y) 3/4,3/4,3/4)

(15) 4' * (0,0,3/4) 1/4,0,z
(4y) 1/4,1/4,3/4)

(16) 4' * (0,0,1/4) -1/4,1/2,z
(4y) 1/4,3/4,1/4)

(17) 4' * (3/4,0,0) x,1/4,0
(4x) 1/4,1/4,1/4)

(18) 4' (0,1/2,1/2) 1/8,y+1/4,y
(2yz) 1/4,3/4,3/4)

(19) 2' 3/8,y+3/4,y
(2yz) 3/4,3/4,3/4)

(20) 4' * (1/4,0,0) x,-1/4,1/2
(4x) 1/4,1/4,3/4)

(21) 4' * (0,1/4,0) 1/2,y,-1/4
(4y) 3/4,1/4,1/4)

(22) 2' (1/2,0,1/2) x-1/4,1/8,x
(2yz) 1/4,1/4,3/4)

(23) 4' * (0,3/4,0) 0,y,1/4
(4y) 1/4,3/4,3/4)

(24) 2' x+3/4,3/8,x
(2yz) 3/4,3/4,3/4)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(2) 2 0,1/4,z
(2y) 1/2,0,0)

(3) 2 1/4,y,0
(4) 2 x,0,1/4

(5) 3' (1/2,1/2,0) x,x,x
(6) 3' (1/6,-1/6,1/6)
(7) 3' (-1/6,1/6,1/6)

(8) 3' (1/6,1/6,-1/6)

(9) 3' (1/2,1/2,1/2) x,x,x
(10) 3' (1/6,-1/6,-1/6)

(11) 3' (-1/6,-1/6,1/6)

(12) 3' (-1/6,1/6,-1/6)

(13) 2' (1/2,1/2,0) x,x+1/4,3/8
(2y) 1/4,3/4,3/4)

(14) 2' x,x+1/4,1/8
(2y) 1/4,1/4,1/4)

(15) 4' * (0,0,1/4) 3/4,0,z
(4y) 1/4,3/4,3/4)

(16) 4' * (0,0,3/4) 1/4,1/2,z

(17) 4' * (1/4,0,0) x,3/4,0
(4x) 1/4,3/4,3/4)

(18) 2' (0,1/2,1/2) 3/8,y-1/4,y
(2yz) 3/4,1/4,3/4)

(19) 2' 1/8,y+1/4,y
(2yz) 1/4,1/4,1/4)

(20) 4' * (3/4,0,0) x,1/4,1/2

(21) 4' * (0,3/4,0) 1/2,y,1/4
(4y) 1/4,3/4,3/4)

(22) 2' (1/2,0,1/2) x+1/4,3/8,x
(2yz) 3/4,3/4,3/4)

(23) 4' * (0,1/4,0) 0,y,3/4
(4y) 3/4,1/4,3/4)

(24) 2' x+1/4,1/8,x
(2yz) 1/4,1/4,1/4)

**Generators selected**

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Site Symmetry.</td>
<td>(0,0,0) + (1/2,1,2/1,2) +</td>
</tr>
<tr>
<td>Multiplicity, Wyckoff letter,</td>
<td></td>
</tr>
<tr>
<td>Generators selected</td>
<td></td>
</tr>
</tbody>
</table>

48 i 1

(1) x,y,z [u,v,w]
(2) x+1/2,y,z+1/2 [u,v,w]
(3) x,y+1/2,z+1/2 [u,v,w]
(4) x+1/2,y+1/2,z [u,v,w]

(5) z,x,y [w,u,v]
(6) z+1/2,x+1/2,y [w,u,v]
(7) z+1/2,x,y+1/2 [w,u,v]
(8) z,x+1/2,y+1/2 [w,u,v]

(9) y,z,x [v,w,u]
(10) y,z+1/2,x+1/2 [v,w,u]
(11) y+1/2,z+1/2,x [v,w,u]
(12) y+1/2,z,x+1/2 [v,w,u]

(13) y+3/4,x+1/4,z+1/4 [v,u,w]
(14) y+3/4,x+3/4,z+3/4 [v,u,w]

(15) y+1/4,x+1/4,z+3/4 [v,u,w]

(16) y+1/4,x+3/4,z+1/4 [v,u,w]

(17) x+3/4,z+1/4,y+1/4 [u,w,v]
(18) x+3/4,z+3/4,y+1/4 [u,w,v]
(19) x+3/4,z+3/4,y+3/4 [u,w,v]

(20) x+1/4,z+1/4,y+3/4 [u,w,v]

(21) z+3/4,y+1/4,x+1/4 [w,v,u]
(22) z+1/4,y+1/4,x+3/4 [w,v,u]
(23) z+1/4,y+3/4,x+1/4 [w,v,u]
(24) z+3/4,y+3/4,x+3/4 [w,v,u]
Symmetry of Special Projections

Along [0,0,1] p4mm'
\( a^* = (a - b)/2 \)
\( b^* = (a + b)/2 \)
Origin at 1/4,0,z

Along [1,1,1] p3m1
\( a^* = (2a - b - c)/3 \)
\( b^* = (-a + 2b - c)/3 \)
Origin at x,x,x

Along [1,1,0] p2'2mm'
\( a^* = c/2 \)
\( b^* = -(-a + b)/2 \)
Origin at x,x,x+1/4,1/8
Origin on 3 [111] at midpoint of three non-intersecting pairs of parallel screw axes 41 and 43 and of three non-intersection pairs of parallel 2 axes.

Asymmetric unit
-3/8 ≤ x ≤ 1/8; -1/8 ≤ y ≤ 1/8; 1/8 ≤ z ≤ 3/8; max(x,y,y - x - 1/8) ≤ z ≤ y+1/4

Vertices

Symmetry Operations

For (0,0,0) + set

1
(1) 1
(1) 0,0,0

(2) 2 (0,0,1/2) 1/4,0,z
(2) 1/2,0,1/2

(3) 2 (0,1/2,0) 0,y,1/4
(3) 0,1/2,1/2

(4) 2 (1/2,0,0) x,1/4,0
(4) 1/2,1/2,0

(5) 3+x,x,x
(3xyz 0,0,0)

(6) 3+ x+1/2,x,x
(3xyz -1 1/2,1/2,0)

(7) 3+ x+1/2, x-1/2,x
(3xyz -1 1/2,0,1/2)

(8) 3+ x,x+1/2,x
(3xyz -1 0,1/2,1/2)

(9) 3- x,x,x
(3xyz -1 0,0,0)

(10) 3- (-1/3,1/3,1/3)
(3xyz -1 0,1/2,1/2)

(11) 3- (1/3,1/3,-1/3)
(3xyz -1 1/2,1/2,0)

(12) 3- (1/3,-1/3,1/3)
(3xyz -1 1/2,0,1/2)
Continued

For $(1/2,1/2,1/2)' +$ set

(1) $t'(1/2,1/2,1/2)$
(2) $2' 0,1/4,z$
(3) $2' 1/4,y,0$
(4) $2' x,0,1/4$

(5) $3' ' (1/2,1/2,1/2) x,x,x$
(6) $3' ' (1/6,-1/6,1/6)$
(7) $3' ' (-1/6,1/6,1/6)$
(8) $3' ' (1/6,1/6,-1/6)$

(9) $3' ' (1/2,1/2,1/2) x,x,x$
(10) $3' ' (1/6,-1/6,-1/6)$
(11) $3' ' (-1/6,-1/6,1/6)$
(12) $3' ' (-1/6,1/6,-1/6)$

(13) $2' (1/2,1/2,0) x,x+1/4,3/8$
(14) $2' x,x+1/4,1/8$
(15) $4' ' (0,0,1/4) 3/4,0,z$
(16) $4' ' (0,0,3/4) 1/4,1/2,z$

(17) $4' ' (1/4,0,0) x,3/4,0$
(18) $2' (0,1/2,1/2) 3/8,y-1/4,y$
(19) $2' 1/8,y+1/4,y$
(20) $4' ' (3/4,0,0) x,1/4,1/2$

(21) $4' ' (0,3/4,0) 1/2,y,1/4$
(22) $2' (1/2,0,1/2) x+1/4,3/8,x$
(23) $4' ' (0,1/4,0) 0,y,3/4$
(24) $2' x+1/4,1/8,x$

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{array}{ccc}
& (0,0,0) + & (1/2,1/2,1/2)' + \\
48 & i & 1 \\
(1) x,y,z [u,v,w] & (2) x+1/2,\bar{y},z+1/2 [u,\bar{v},\bar{w}] & (3) x,y+1/2,z+1/2 [u,v,w] \\
(5) z,x,y [w,u,v] & (6) z+1/2,x+1/2,\bar{y} [w,\bar{u},\bar{v}] & (7) \bar{z}+1/2,x,y+1/2 [\bar{w},u,v] \\
(9) y,z,x [v,w,u] & (10) \bar{y},z+1/2,x+1/2 [\bar{v},w,\bar{u}] & (11) y+1/2,\bar{z}+1/2,x [v,w,u] \\
(13) y+3/4,x+1/4,\bar{z}+1/4 [v,u,w] & (14) \bar{y}+3/4,\bar{x}+3/4,z+3/4 [\bar{v},\bar{u},\bar{w}] & (15) y+1/4,x+1/4,z+3/4 [v,u,w] \\
(17) x+3/4,z+1/4,y+1/4 [u,w,v] & (18) x+1/4,z+3/4,y+1/4 [u,w,v] & (19) x+3/4,z+3/4,y+3/4 [u,w,v] \\
(21) z+3/4,y+1/4,x+1/4 [w,v,u] & (22) z+1/4,y+1/4,x+3/4 [w,v,u] & (23) \bar{z}+1/4,y+3/4,x+1/4 [\bar{w},v,u] \\
\end{array}
\]
Continued


24 f 2'.2' x, 0, 1/4 [u, 0, u] x+1/2, 0, 3/4 [u, 0, u] 1/4, x, 0 [0, u, 0] 3/4, x+1/2, 0 [0, u, 0] 0, 1/4, x [0, 0, u] 3/4, x+1/2, 0 [0, u, 0] 3/4, x+1/2, 1/4 [0, 0, u] 0, 1/4, x+1/4, 0 [0, u, 0] 1/2, 1/4, x+3/4 [0, u, 0] x+1/2, x, 1/4 [u, u, u] x+3/4, x+1/2, x [u, u, u] x+3/4, x+1/4, x+1/4 [u, u, u] x+1/4, x+1/2, x+3/4 [u, u, u]

16 e .3'. x, x, x [u, u, u] x+1/2, x, 1/2 [u, u, u] x+1/2, x+1/2, x [u, u, u] x+3/4, x+1/4, x+3/4 [u, u, u] x+1/4, x+1/4, x+3/4 [u, u, u] x+1/4, x+3/4, x+3/4 [u, u, u]

12 d 2'.22' 5/8, 0, 1/4 [0, v, v] 7/8, 0, 3/4 [0, v, v] 1/4, 5/8, 0 [v, 0, v] 3/4, 7/8, 0 [v, 0, v] 0, 1/4, 5/8 [v, v, 0] 0, 3/4, 7/8 [v, v, 0]

12 c 2'.22' 1/8, 0, 1/4 [0, v, v] 3/8, 0, 3/4 [0, v, v] 1/4, 1/8, 0 [v, v, 0] 3/4, 3/8, 0 [v, 0, v] 0, 1/4, 1/8 [v, v, 0] 0, 3/4, 3/8 [v, v, 0]

8 b .32' 7/8, 7/8, 7/8 [0, 0, 0] 5/8, 1/8, 3/8 [0, 0, 0] 1/8, 3/8, 5/8 [0, 0, 0] 3/8, 5/8, 1/8 [0, 0, 0]


Symmetry of Special Projections

Along [0, 0, 1] p_4' 4m'm'

a* = (a - b)/2

b* = (a + b)/2

Origin at 1/4, 0, z

Along [1, 1, 1] p3m11'

a* = (2a - b - c)/3

b* = (-a + 2b - c)/3

Origin at x, x, x

Along [1, 1, 0] p_2'' 2m'm'

a* = c/2

b* = -(a + b)/2

Origin at x, x+1/4, 1/8

Asymmetric unit
-3/8 ≤ x ≤ 1/8; -1/8 ≤ y ≤ 1/8; 1/8 ≤ z ≤ 3/8; max(x,y,y - x - 1/8) ≤ z ≤ y+1/4

Vertices

Symmetry Operations
For (0,0,0) + set

(1) 1
(2) 2 (0,0,1/2) 1/4,0,z
(3) 2 (0,1/2,0) 0,y,1/4
(4) 2 (1/2,0,0) x,1/4,0
(2z) 1/2,0,1/2
(2y) 0,1/2,1/2
(2x) 1/2,1/2,0

(5) 3^+ x,x,x
(6) 3^- x+1/2,x,x
(3xyz^-1) 1/2,1/2,0

(9) 3^- x,x,x
(10) 3^- (-1/3,1/3,1/3) x+1/6,x +1/6,x
(3xyz^-1) 0,1/2,1/2
(3x) 1/2,1/2,0

(11) 3^- (1/3,1/3,-1/3) x+1/3,x +1/6,x
(3xyz^-1) 1/2,1/2,0
(3x) 1/2,0,1/2
Continued

(13) $2' (1/2, 1/2, 0)$ $x, x'-1/4, 1/8$

(14) $2' x, x+3/4, 3/8$

(15) $4' (0, 0, 3/4) 1/4, 0, z$

(16) $4' (0, 0, 1/4) -1/4, 1/2, z$

(17) $4' (3/4, 0, 0) x, 1/4, 0$

(18) $2' (0, 1/2, 1/2) 1/8, y+1/4, y$

(19) $2' 3/8, y+3/4, y$

(20) $4' (1/4, 0, 0) x, -1/4, 1/2$

(21) $4' (0, 1/4, 0) 1/2, y, -1/4$

For $(1/2, 1/2, 1/2') +$ set

(1) $t' (1/2, 1/2, 1/2)$

(2) $2' 0, 1/4, z$

(3) $2' 1/4, y, 0$

(4) $2' x, 0, 1/4$

(5) $3' (1/2, 1/2, 1/2) x, x, x$

(6) $3' (1/6, -1/6, 1/6)$

(7) $3' (-1/6, 1/6, 1/6)$

(8) $3' (1/6, 1/6, -1/6)$

(3) $x, y, z$

(2) $1/4, 1/4, 1/4$

(4) $1/4, 3/4, 3/4$

(17) $4' (1/4, 0, 0) x, 3/4, 0$

(18) $2' (0, 1/2, 1/2) 3/8, y-1/4, y$

(19) $2' 1/8, y-1/4, y$

(20) $4' (3/4, 0, 0) x, 1/4, 1/2$

(21) $4' (0, 3/4, 0) 1/2, y, 1/4$

(22) $2' (1/2, 0, 1/2) x+1/4, 3/8, x$

(23) $4' (0, 1/4, 0) 0, y, 3/4$

(24) $2' x+1/4, 1/8, x$

Generators selected

(1); $t(1, 0, 0); t(0, 1, 0); t'(1/2, 1/2, 1/2); (2); (3); (5); (13).

Positions

Multiplicity: 48

Wyckoff letter: i

Site Symmetry: $1$

Positions selected

$\mathbf{(0,0,0)} + (1/2, 1/2, 1/2') +$

Coordinates

(1) $x, y, z [u, v, w]$

(2) $\bar{x} + 1/2, \bar{y}, z+1/2 [u, v, w]$

(3) $x, y+1/2, z+1/2 [u, v, w]$

(4) $x+1/2, y+1/2, z [u, v, w]$

(5) $z, x, y [w, u, v]$

(6) $z+1/2, x+1/2, \bar{y} [w, u, v]$

(7) $z+1/2, x, y+1/2 [w, u, v]$

(8) $z, x+1/2, y+1/2 [w, u, v]$

(9) $y, z, x [v, w, u]$

(10) $\bar{y}, z+1/2, x+1/2 [v, w, u]$

(11) $y+1/2, z+1/2, x [v, w, u]$

(12) $\bar{y}+1/2, z, x+1/2 [v, w, u]$

(13) $y+3/4, x+1/4, z+1/4 [v, w, u]$

(14) $\bar{y}+3/4, x+3/4, z+3/4 [v, w, u]$

(15) $y+1/4, x+1/4, z+3/4 [v, w, u]$

(16) $\bar{y}+1/4, x+3/4, z+1/4 [v, w, u]$

(17) $x+3/4, z+1/4, y+1/4 [u, w, v]$

(18) $x+1/4, z+3/4, y+1/4 [u, w, v]$

(19) $x+3/4, z+3/4, y+3/4 [u, w, v]$

(20) $x+1/4, z+1/4, y+3/4 [u, w, v]$

(21) $z+3/4, y+1/4, x+1/4 [w, v, u]$

(22) $z+1/4, y+3/4, x+3/4 [w, v, u]$

(23) $\bar{z}+1/4, y+3/4, x+1/4 [w, v, u]$

(24) $\bar{z}+3/4, y+3/4, x+3/4 [w, v, u]$

214.5.1571 - 2 - 3540
Symmetry of Special Projections

Along [0,0,1] \( p_{0\nu} 4'mm' \)
\( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)
Origin at 1/4,0,z

Along [1,1,1] \( p3m11' \)
\( a^* = (2a - b - c)/3 \) \( b^* = (-a + 2b - c)/3 \)
Origin at x,x,x

Along [1,1,0] \( p_{2\nu} 2m'm' \)
\( a^* = (-a + b)/2 \) \( b^* = c/2 \)
Origin at x,x+1/4,5/8
Origin at $\overline{43m}$

Asymmetric unit

\begin{align*}
0 \leq x \leq 1; & \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min(x, 1-x); \quad z \leq y \\
\text{Vertices} & \quad 0,0,0 \quad 1,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2
\end{align*}

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
& \quad (1,0,0) \\
(5) & \quad 3^+ \ x,x,x \\
& \quad (3_{xyz}^{1},0,0,0) \\
(9) & \quad 3^- \ x,x,x \\
& \quad (3_{xyz}^{1},0,0,0) \\
(2) & \quad 2 \ 0,0,z \quad (2z,0,0,0) \\
(6) & \quad 3^+ \ x,x,x \\
& \quad (3_{xyz}^{1},0,0,0) \\
(10) & \quad 3^+ \ x,x,x \\
& \quad (3_{xyz}^{1},0,0,0) \\
(3) & \quad 2 \ 0,y,0 \quad (2y,0,0,0) \\
(7) & \quad 3^+ \ x,x,x \\
& \quad (3_{xyz}^{1},0,0,0) \\
(11) & \quad 3^- \ x,x,x \quad (3_{xyz}^{1},0,0,0) \\
(4) & \quad 2 \ x,0,0 \quad (2z,0,0,0) \\
(8) & \quad 3^+ \ x,x,x \\
& \quad (3_{xyz}^{1},0,0,0) \\
(12) & \quad 3^- \ x,x,x \quad (3_{xyz}^{1},0,0,0)
\end{align*}

\textit{215.1.1572 - 1 - 3542}
Continued 215.1.1572 P4 \textsuperscript{3}m

(13) m x,x,z \\
\text{(m}_{xy}\big|0,0,0) \\
(14) m x,x,z \\
\text{(m}_{xy}\big|0,0,0) \\
(15) \text{4}^{+} 0,0,z; 0,0,0 \\
\text{(4}_{z}\big|0,0,0) \\
(16) \text{4}^{-} 0,0,z; 0,0,0 \\
\text{(4}_{z}^{-}\big|0,0,0) \\
(17) m x,y,y \\
\text{(m}_{yz}\big|0,0,0) \\
(18) \text{4}^{+} x,0,0; 0,0,0 \\
\text{(4}_{y}\big|0,0,0) \\
(19) \text{4}^{-} x,0,0; 0,0,0 \\
\text{(4}_{y}^{-}\big|0,0,0) \\
(20) m x,y,y \\
\text{(m}_{yz}\big|0,0,0) \\
(21) m x,y,x \\
\text{(m}_{xz}\big|0,0,0) \\
(22) \text{4}^{-} 0,y,0; 0,0,0 \\
\text{(4}_{x}^{-}\big|0,0,0) \\
(23) m x,y,x \\
\text{(m}_{xz}\big|0,0,0) \\
(24) \text{4}^{+} 0,y,0; 0,0,0 \\
\text{(4}_{y}\big|0,0,0) \\

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>24</th>
<th>j</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z ([u,v,w])</td>
<td>(2) \text{x},\text{y},z ([u,v,w])</td>
<td>(3) \text{x},\text{y},z ([u,v,w])</td>
</tr>
<tr>
<td>(5) z,x,y ([w,u,v])</td>
<td>(6) z,x,y ([w,u,v])</td>
<td>(7) \text{z},z,x ([w,u,v])</td>
</tr>
<tr>
<td>(9) y,z,x ([v,w,u])</td>
<td>(10) y,z,x ([v,w,u])</td>
<td>(11) \text{y},z,x ([v,w,u])</td>
</tr>
<tr>
<td>(13) x,z,y ([u,w,v])</td>
<td>(14) x,z,y ([u,w,v])</td>
<td>(15) \text{y},x,z ([v,u,w])</td>
</tr>
<tr>
<td>(17) x,z,y ([u,w,v])</td>
<td>(18) x,z,y ([u,w,v])</td>
<td>(19) \text{x},\text{y},z ([u,w,v])</td>
</tr>
<tr>
<td>(21) x,y,x ([w,v,u])</td>
<td>(22) \text{z},\text{y},\text{x} ([w,v,u])</td>
<td>(23) \text{z},\text{y},\text{x} ([w,v,u])</td>
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<tr>
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<td>x,x,z ([u,u,0])</td>
<td>x,x,z ([u,u,0])</td>
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<tr>
<td>z,x,x ([0,u,0])</td>
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<td>z,x,x ([0,u,0])</td>
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<tbody>
<tr>
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<td>x,1/2,0 ([u,0,0])</td>
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<td>1/2,0,x ([0,u,0])</td>
<td>1/2,0,x ([0,u,0])</td>
<td>1/2,x,0 ([0,u,0])</td>
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<td>x,0,1/2 ([u,0,0])</td>
<td>x,0,1/2 ([u,0,0])</td>
<td>0,1/2,x ([0,u,0])</td>
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<tbody>
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<td>1/2,x,1/2 ([0,0,0])</td>
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<tr>
<td>1/2,1/2,0 ([0,0,0])</td>
<td>1/2,1/2,0 ([0,0,0])</td>
<td>1/2,1/2,x ([0,0,0])</td>
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<th>2.mm</th>
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<td>x,0,0 ([0,0,0])</td>
<td>0,x,0 ([0,0,0])</td>
</tr>
<tr>
<td>0,0,0 ([0,0,0])</td>
<td>0,0,0 ([0,0,0])</td>
<td>0,0,x ([0,0,0])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4</th>
<th>e</th>
<th>.3m</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x,x ([0,0,0])</td>
<td>x,x,x ([0,0,0])</td>
<td>x,x,x ([0,0,0])</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>3</th>
<th>d</th>
<th>4.mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2,0,0 ([0,0,0])</td>
<td>1/2,0,0 ([0,0,0])</td>
<td>0,1/2,0 ([0,0,0])</td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Group</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4m'</td>
<td>( a^* = a ) ( b^* = b ) ( c^* = \frac{1}{2},1/2,1/2 ) ( {0,0,0} ) ( 1/2,1/2,1/2 ) ( {0,0,0} )</td>
</tr>
<tr>
<td>Along [1,1,1]</td>
<td>p31m</td>
<td>( a^* = \frac{1}{2}(2a - b - c) ) ( b^* = \frac{1}{2}(-a + 2b - c) )</td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>p1m11'</td>
<td>( a^* = (a + b)/2 ) ( b^* = c )</td>
</tr>
</tbody>
</table>

Origin at 0,0,z Origin at x,x,x Origin at x,x,0
Origin at \( \overline{4}3m1' \)

Asymmetric unit

\[
0 \leq x \leq 1; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq \min(x, 1-x); \quad z \leq y
\]

Vertices

\[
(0,0,0) \quad (1,0,0) \quad (1/2,1/2,0) \quad (1/2,1/2,1/2)
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2) & \quad (2,0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(3) & \quad (2,0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(4) & \quad (2,0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
(6) & \quad (3_{xyz}^{-1}|0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
(7) & \quad (3_{xyz}^{-1}|0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
(8) & \quad (3_{xyz}^{-1}|0,0,0) \\
(9) & \quad 3^- \quad x,x,x \\
(9) & \quad (3_{xyz}^{-1}|0,0,0) \\
(10) & \quad 3^- \quad x,x,x \\
(10) & \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^- \quad x,x,x \\
(11) & \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^- \quad x,x,x \\
(12) & \quad (3_{xyz}|0,0,0)
\end{align*}
\]
Continued

<table>
<thead>
<tr>
<th>215.2.1573</th>
<th>P4 3m1'</th>
</tr>
</thead>
</table>

(13) m x,x,z  
(m x y \(0,0,0\))  

(14) m x,x,z  
(m x y \(0,0,0\))  

(15) m x,x,z  
(m x y \(0,0,0\))  

(16) m x,x,z  
(m x y \(0,0,0\))  

(17) m x,y,y  
(m y z \(0,0,0\))  

(18) m x,y,y  
(m y z \(0,0,0\))  

(19) m x,y,y  
(m y z \(0,0,0\))  

(20) m x,y,y  
(m y z \(0,0,0\))  

(21) m x,y,x  
(m z x \(0,0,0\))  

(22) m x,y,x  
(m z x \(0,0,0\))  

(23) m x,y,x  
(m z x \(0,0,0\))  

(24) m x,y,x  
(m z x \(0,0,0\))  

For 1' + set

(1) 1'  
(1 | 0,0,0)  

(2) 2' 0,0,z  
(2 | 0,0,0)  

(3) 2' 0,y,0  
(2 | 0,0,0)  

(4) 2' 0,x,0  
(2 | 0,0,0)  

(5) 3' x,x,x  
(3 x y z \(0,0,0\))  

(6) 3' x,x,x  
(3 x y z \(0,0,0\))  

(7) 3' x,x,x  
(3 x y z \(0,0,0\))  

(8) 3' x,x,x  
(3 x y z \(0,0,0\))  

(9) 3' x,x,x  
(3 x y z \(0,0,0\))  

(10) 3' x,x,x  
(3 x y z \(0,0,0\))  

(11) 3' x,x,x  
(3 x y z \(0,0,0\))  

(12) 3' x,x,x  
(3 x y z \(0,0,0\))  

(13) m' x,x,z  
(m x y \(0,0,0\))  

(14) m' x,x,z  
(m x y \(0,0,0\))  

(15) m' x,x,z  
(m x y \(0,0,0\))  

(16) m' x,x,z  
(m x y \(0,0,0\))  

(17) m' x,y,y  
(m y z \(0,0,0\))  

(18) m' x,y,y  
(m y z \(0,0,0\))  

(19) m' x,y,y  
(m y z \(0,0,0\))  

(20) m' x,y,y  
(m y z \(0,0,0\))  

(21) m' x,y,x  
(m z x \(0,0,0\))  

(22) m' x,y,x  
(m z x \(0,0,0\))  

(23) m' x,y,x  
(m z x \(0,0,0\))  

(24) m' x,y,x  
(m z x \(0,0,0\))  

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 j 11'</td>
<td></td>
</tr>
</tbody>
</table>

(1) x,y,z \([0,0,0]\)  

(2) x,y,z \([0,0,0]\)  

(3) x,y,z \([0,0,0]\)  

(4) x,y,z \([0,0,0]\)  

(5) z,x,y \([0,0,0]\)  

(6) z,x,y \([0,0,0]\)  

(7) z,x,y \([0,0,0]\)  

(8) z,x,y \([0,0,0]\)  

(9) y,z,x \([0,0,0]\)  

(10) y,z,x \([0,0,0]\)  

(11) y,z,x \([0,0,0]\)  

(12) y,z,x \([0,0,0]\)  

(13) y,x,z \([0,0,0]\)  

(14) y,x,z \([0,0,0]\)  

(15) y,x,z \([0,0,0]\)  

(16) y,x,z \([0,0,0]\)  

(17) x,z,y \([0,0,0]\)  

(18) x,z,y \([0,0,0]\)  

(19) x,z,y \([0,0,0]\)  

(20) x,z,y \([0,0,0]\)  

(21) z,y,x \([0,0,0]\)  

(22) z,y,x \([0,0,0]\)  

(23) z,y,x \([0,0,0]\)  

(24) z,y,x \([0,0,0]\)  

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Symmetry of Special Projections

Along [0,0,1] \( p4mm1' \) \( a^* = a \quad b^* = b \) Origin at 0,0,z
Along [1,1,1] \( p31m1' \) \( a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \) Origin at x,x,x
Along [1,1,0] \( p1m1' \) \( a^* = (-a + b)/2 \quad b^* = c \) Origin at x,x,0
Origin at $\overline{4}3m'$

Asymmetric unit:

\[
\begin{align*}
0 & \leq x \leq 1; \\
0 & \leq y \leq 1/2; \\
0 & \leq z \leq 1/2; \\
y & \leq \min(x, 1-x); \\
z & \leq y
\end{align*}
\]

Vertices:

\[
\begin{align*}
0,0,0 & \\
1,0,0 & \\
1/2,1/2,0 & \\
1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations:

\[
\begin{align*}
(1) & \ 1 \\
(2) & \ 2 0,0,z \\
(3) & \ 2 0,y,0 \\
(4) & \ 2 x,0,0 \\
(5) & \ 3^+ x,x,x \\
(6) & \ 3^+ x,x,x \\
(7) & \ 3^+ x,x,x \\
(8) & \ 3^+ x,x,x \\
(9) & \ 3^- x,x,x \\
(10) & \ 3^- x,x,x \\
(11) & \ 3^- x,x,x \\
(12) & \ 3^- x,x,x \\
(3_{xyz}) & \ |0,0,0|
\end{align*}
\]
Continued 215.3.1574

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 j 1</td>
<td>1</td>
</tr>
<tr>
<td>12 i ..m’</td>
<td>2.. x,1/2,0 [0,u,0] 0,x,1/2 [0,u,0] 0,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td>12 h 2..</td>
<td>2.m’m’ x,0,0 [0,u,0] x,0,0 [0,u,0] 0,x,0 [0,u,0]</td>
</tr>
<tr>
<td>6 f 2.m’m’</td>
<td>x,0,0 [0,u,0] x,0,0 [0,u,0] 0,x,0 [0,u,0]</td>
</tr>
<tr>
<td>4 e .3m’</td>
<td>x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]</td>
</tr>
<tr>
<td>3 d 4’.2.m’</td>
<td>1/2,0,0 [0,0,0] 0,1/2,0 [0,0,0] 0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>
Continued

\[ \begin{array}{ccc}
3 & c & 4'2.m' \ 0,1/2,1/2 [0,0,0] \\
1 & b & 4'3m' \ 1/2,1/2,1/2 [0,0,0] \\
1 & a & 4'3m' \ 0,0,0 [0,0,0]
\end{array} \]

**Symmetry of Special Projections**

**Along [0,0,1]** \( p4m'm' \)

\[ \begin{array}{ccc}
a^* &=& a \\
b^* &=& b
\end{array} \]

Origin at 0,0,z

**Along [1,1,1]** \( p31m' \)

\[ \begin{array}{ccc}
a^* &=& (2a - b - c)/3 \\
b^* &=& (-a + 2b - c)/3
\end{array} \]

Origin at x,x,x

**Along [1,1,0]** \( p1m'1 \)

\[ \begin{array}{ccc}
a^* &=& (-a + b)/2 \\
b^* &=& c
\end{array} \]

Origin at x,x,0
Origin at $\overline{4}3m$

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq 1/2$; $0 \leq z \leq 1/2$; $y \leq \min(x,1-x)$; $z \leq y$

Vertices $0,0,0$ $1,0,0$ $1/2,1/2,0$ $1/2,1/2,1/2$

Symmetry Operations

For $(0,0,0) +$ set

1. $1$
   
2. $2$ 0,0,$z$
   
3. $2$ 0,$y,0$
   
4. $2$ $x,0,0$

For $(1,0,0)' +$ set

1. $t'$ (1,0,0)
   
2. $2'$ 1/2,0,$z$
   
3. $2'$ 1/2,$y,0$
   
4. $2'$ (1,0,0) $x,0,0$

Generators selected $(1); t'(1,0,0); t'(0,0,1); t'(0,1,0); (2); (3); (5); (13).
Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1,0,0)' +</td>
</tr>
</tbody>
</table>

48  j  1

(1) x,y,z [u,v,w]  (2) x, y, z [u, v, w]  (3) x, y, z [u, v, w]  (4) x, y, z [u, v, w]
(5) z,x,y [w,u,v]  (6) z, x, y [w, u, v]  (7) z, x, y [w, u, v]  (8) z, x, y [w, u, v]
(9) y,z,x [v,w,u]  (10) y, z, x [v, w, u]  (11) y, z, x [v, w, u]  (12) y, z, x [v, w, u]
(13) y,x,z [v,u,w]  (14) y, x, z [v, u, w]  (15) y, x, z [v, u, w]  (16) y, x, z [v, u, w]
(17) x,y,z [u,v,w]  (18) x, y, z [u, v, w]  (19) x, y, z [u, v, w]  (20) x, y, z [u, v, w]
(21) z,y,x [w,u,v]  (22) z, y, x [w, u, v]  (23) z, y, x [w, u, v]  (24) z, y, x [w, u, v]

24  i  .m  24  i  .m

x,x,z [u,u,0]  x, x, z [u, u, 0]  x, x, z [u, u, 0]  x, x, z [u, u, 0]

z,x,x [0,u,u]  z, x, x [0, u, u]  z, x, x [0, u, u]  z, x, x [0, u, u]

x,z,x [u,0,u]  x, z, x [u, 0, u]  x, z, x [u, 0, u]  x, z, x [u, 0, u]

24  h  2'..  24  h  2'..

x,1/2,0 [0,v,w]  0,x,1/2 [w,0,v]  0,x,1/2 [w,0,v]  0,x,1/2 [w,0,v]

1/2,0,x [v,w,0]  1/2,0,x [v, w, 0]  1/2,0,x [v, w, 0]  1/2,0,x [v, w, 0]

x,0,1/2 [0,w,v]  0,1/2,x [w, v, 0]  0,1/2,x [w, v, 0]  0,1/2,x [w, v, 0]

12  g  2.mm  12  g  2.mm

x,1/2,1/2 [0,0,0]  x, 1/2,1/2 [0,0,0]  1/2,x,1/2 [0,0,0]  1/2,x,1/2 [0,0,0]

1/2,x,1/2 [0,0,0]  1/2,1/2,x [0,0,0]  1/2,1/2,x [0,0,0]  1/2,1/2,x [0,0,0]

12  f  2.mm  12  f  2.mm

x,0,0 [0,0,0]  x, 0,0 [0,0,0]  0,x,0 [0,0,0]  0,x,0 [0,0,0]

0,x,0 [0,0,0]  0,0,x [0,0,0]  0,0,x [0,0,0]  0,0,x [0,0,0]

8  e  .3m  8  e  .3m

x,x,x [0,0,0]  x, x, x [0,0,0]  x, x, x [0,0,0]  x, x, x [0,0,0]

2  b  43m  2  b  43m

1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]  1/2,1/2,1/2 [0,0,0]

2  a  43m  2  a  43m

0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1] p4mm1'  Along [1,1,1] p31m1'  Along [1,1,0] p1m11'

\[ \mathbf{a}^* = \mathbf{a} \] \[ \mathbf{b}^* = \mathbf{b} \] \[ \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \] \[ \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3 \] \[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \] \[ \mathbf{b}^* = \mathbf{c} \]

Origin at 0,0,z  Origin at x,x,x  Origin at x,x,0
Origin at $\overline{4}3m$

Asymmetric unit

\[0 < x < 1; \quad 0 < y < 1/2; \quad 0 < z < 1/2; \quad y \leq \min(x,1-x); \quad z \leq y\]

Vertices

\[0,0,0 \quad 1,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2\]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad 1 \\
(1 | 0,0,0) & \quad (2) & \quad 2 \quad 0,0,z \\
& & \quad (2_z | 0,0,0) \\
(5) & \quad 3^+ \ x,x,x \\
(3_{xyz} | 0,0,0) & \quad (6) & \quad 3^+ \ x,x,x \\
& & \quad (3_{xyz}^{-1} | 0,0,0) \\
(9) & \quad 3^- \ x,x,x \\
(3_{xyz}^{-1} | 0,0,0) & \quad (10) & \quad 3^- \ x,x,x \\
& & \quad (3_{xyz} | 0,0,0) \\
(13) & \quad m' \ x,x,z \\
(m_{yz} | 0,0,0)' & \quad (14) & \quad m' \ x,x,z \\
& & \quad (m_{xy} | 0,0,0)' \\
(17) & \quad m' \ x,y,y \\
(m_{yz}^{-1} | 0,0,0)' & \quad (18) & \quad 4^- \ x,0,0; 0,0,0 \\
& & \quad (4_x | 0,0,0)' \\
(21) & \quad m' \ x,y,x \\
(m_{xz}^{-1} | 0,0,0)' & \quad (22) & \quad 4^- \ y,0,0; 0,0,0 \\
& & \quad (4_y | 0,0,0)' \\
(1) & \quad t'(1,0,0) \\
(1 | 1,0,0)' & \quad (2) & \quad 2' \ 1/2,0,0 \\
& & \quad (2_z | 1,0,0)' \\
(5) & \quad 3^- \ (1/3,1/3,1/3) \\
(3_{xyz} | 0,0,0)' & \quad (6) & \quad 3^- \ (1/3,1/3,1/3) \\
& & \quad (3_{xyz}^{-1} | 1,0,0)' \\
(9) & \quad 3^- \ (1/3,1/3,1/3) \\
(3_{xyz}^{-1} | 1,0,0)' & \quad (10) & \quad 3^- \ (1/3,1/3,1/3) \\
& & \quad (3_{xyz} | 1,0,0)' \\
(13) & \quad g(1/2,1/2,0) \ x+1/2,x,z \\
(m_{xy} | 0,0,0) & \quad (14) & \quad g(1/2,1/2,0) \ x+1/2,x,z \\
& & \quad (m_{xy} | 1,0,0) \\
(17) & \quad a(1,0,0) \ x,y,y \\
(m_{yz} | 0,0,0) & \quad (18) & \quad 4^- \ x+1/2,0,0; 1/2,0,0 \\
& & \quad (4_x | 1,0,0) \\
(21) & \quad g(1/2,1/2,0) \ x+1/2,y,x \\
(m_{xz} | 0,0,0) & \quad (22) & \quad 4^- \ y,1/2,-1/2; 1/2,0,1/2 \\
& & \quad (4_y | 1,0,0) \\
\end{align*}
\]

For \((1,0,0)'\) + set

\[
\begin{align*}
(1) & \quad t'(1,0,0) \\
(1 | 1,0,0) & \quad (2) & \quad 2' \ 1/2,0,0 \\
& & \quad (2_z | 1,0,0)' \\
(5) & \quad 3^- \ (1/3,1/3,1/3) \\
(3_{xyz}^{-1} | 0,0,0)' & \quad (6) & \quad 3^- \ (1/3,1/3,1/3) \\
& & \quad (3_{xyz}^{-1} | 1,0,0)' \\
(9) & \quad 3^- \ (1/3,1/3,1/3) \\
(3_{xyz}^{-1} | 1,0,0)' & \quad (10) & \quad 3^- \ (1/3,1/3,1/3) \\
& & \quad (3_{xyz} | 1,0,0)' \\
(13) & \quad g(1/2,1/2,0) \ x+1/2,x,z \\
(m_{xy} | 0,0,0) & \quad (14) & \quad g(1/2,1/2,0) \ x+1/2,x,z \\
& & \quad (m_{xy} | 1,0,0) \\
(17) & \quad a(1,0,0) \ x,y,y \\
(m_{yz} | 0,0,0) & \quad (18) & \quad 4^- \ x+1/2,0,0; 1/2,0,0 \\
& & \quad (4_x | 1,0,0) \\
(21) & \quad g(1/2,1/2,0) \ x+1/2,y,x \\
(m_{xz} | 0,0,0) & \quad (22) & \quad 4^- \ y,1/2,-1/2; 1/2,0,1/2 \\
& & \quad (4_y | 1,0,0) \\
\end{align*}
\]

Generators selected

\(1); \ t'(1,0,0); \ t'(0,0,1); \ t'(0,0,1); \ (2); \ (3); \ (5); \ (13).\)
Positions

Multiplicity, Wyckoff letter, Site Symmetry.

$$\begin{align*}
\text{Positions} & \quad \text{Coordinates} \\
(0,0,0) & + \quad (1,0,0)' + \\
\end{align*}$$

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>_mob_1</th>
<th>Wyckoff letter</th>
<th>_mob_2</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>j</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(1) x,y,z [u,v,w]  
(2) $\bar{x},\bar{y},\bar{z} [\bar{u},\bar{v},\bar{w}]$  
(3) $x,y,z [u,v,w]$  
(4) $x,y,z [u,v,w]$  

(5) z,x,y [w,u,v]  
(6) $\bar{z},\bar{x},\bar{y} [\bar{w},\bar{u},\bar{v}]$  
(7) $z,x,y [w,u,v]$  
(8) $z,x,y [w,u,v]$  

(9) y,z,x [v,w,u]  
(10) $\bar{y},\bar{z},\bar{x} [\bar{v},\bar{w},\bar{u}]$  
(11) $y,z,x [v,w,u]$  
(12) $y,z,x [v,w,u]$  

(13) y,x,z [v,u,w]  
(14) $\bar{y},\bar{x},\bar{z} [\bar{v},\bar{u},\bar{w}]$  
(15) $y,x,z [v,u,w]$  
(16) $y,x,z [v,u,w]$  

(17) x,z,y [w,u,v]  
(18) $\bar{x},\bar{z},\bar{y} [\bar{w},\bar{u},\bar{v}]$  
(19) $x,z,y [w,u,v]$  
(20) $x,z,y [w,u,v]$  

(21) z,y,x [w,v,u]  
(22) $\bar{z},\bar{y},\bar{x} [\bar{w},\bar{v},\bar{u}]$  
(23) $z,y,x [w,v,u]$  
(24) $z,y,x [w,v,u]$  

24 i ...m' x,x,z [u,u,w]  
$x,x,z [u,u,w]$  
$z,x,x [w,u,u]$  
$\bar{z},\bar{x},\bar{z} [\bar{w},\bar{u},\bar{u}]$  
$\bar{z},\bar{x},\bar{z} [\bar{w},\bar{u},\bar{u}]$  

24 h 2'.. x,1/2,0 [0,v,w]  
$x,1/2,0 [0,v,w]$  
$0,x,1/2 [w,0,v]$  
$0,x,1/2 [w,0,v]$  

12 g 2.m'm' x,1/2,1/2 [u,0,0]  
$x,1/2,1/2 [u,0,0]$  
$1/2,x,1/2 [0,u,0]$  
$1/2,x,1/2 [0,u,0]$  

12 f 2.mm x,0,0 [u,0,0]  
$x,0,0 [u,0,0]$  
$0,x,0 [0,u,0]$  
$0,x,0 [0,u,0]$  

8 e .3m x,x,x [u,u,u]  
$x,x,x [u,u,u]$  
$x,x,x [u,u,u]$  
$x,x,x [u,u,u]$  

6 d 42'.m' 1/2,0,0 [u,0,0]  
$0,1/2,0 [u,0,0]$  
$0,1/2,0 [u,0,0]$  
$0,1/2,0 [u,0,0]$  

6 c 42'.m' 1/2,1/2,0 [u,0,0]  
$0,1/2,0 [u,0,0]$  
$0,1/2,0 [u,0,0]$  
$0,1/2,0 [u,0,0]$  

2 b 43'm' 1/2,1/2,1/2 [0,0,0]  
$1/2,1/2,0 [0,0,0]$  
$1/2,1/2,0 [0,0,0]$  
$1/2,1/2,0 [0,0,0]$  

2 a 43'm' 0,0,0 [0,0,0]  
$0,0,0 [0,0,0]$  
$0,0,0 [0,0,0]$  
$0,0,0 [0,0,0]$  

Symmetry of Special Projections

Along [0,0,1] p4mm1

<table>
<thead>
<tr>
<th>a* = a</th>
<th>b* = b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
</tr>
</tbody>
</table>

Along [1,1,1] p31m1

<table>
<thead>
<tr>
<th>a* = (2a - b - c)/3</th>
<th>b* = (-a + 2b - c)/3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at x,x,x</td>
<td></td>
</tr>
</tbody>
</table>

Along [1,1,0] p21m1

<table>
<thead>
<tr>
<th>a* = (-a + b)/2</th>
<th>b* = c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Origin at x-1/4,x+1/4,0</td>
<td></td>
</tr>
</tbody>
</table>

215.5.1576 - 3 - 3556
Origin at $\overline{4}3m$

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad -y \leq z \leq y \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4 \]

Symmetry Operations

For $(0,0,0) + \text{set}$

(1) 1

(5) $3^{+} x,x,x$

(9) $3^{+} x,x,x$

(2) $2 \quad 0,0,z$

(6) $3^{+} x,x,x$

(10) $3^{+} x,x,x$

(3) $2 \quad 0,y,0$

(7) $3^{+} x,x,x$

(11) $3^{+} x,x,x$

(4) $2 \quad x,0,0$

(8) $3^{+} x,x,x$

(12) $3^{+} x,x,x$
For $0,1/2,1/2$ + set

For $1/2,0,1/2$ + set

216.1.1577 - 2 - 3558
Continued

For (1/2,1/2,0) + set

| (1) t(1/2,1/2,0) | (2) 2 1/4,1/4,z | (3) 2 (0,1/2,0) 1/4,y,0 | (4) 2 (1/2,0,0) x,1/4,0 |
| (1) | 1/2,1/2,0) | (2) 1/2,1/2,0) | (3) 1/2,1/2,0) | (4) 1/2,1/2,0) |

(5) 3* (1/3,1/3,1/3) x+1/6,x+1/3,x (3,xyz | 1/2,1/2,0) | (6) 3* x+1/2,x,x (7) 3* x+1/2,x,x (8) 3* (1/3,1/3,-1/3) x+1/6,x+1/3,x (3,xyz | 1/2,1/2,0) |

(9) 3* (1/3,1/3,1/3) x+1/3,x+1/6,x (3,xyz | 1/2,1/2,0) | (10) 3* x,x+1/2,x (11) 3* (1/3,1/3,-1/3) x+1/3,x+1/6,x (3,xyz | 1/2,1/2,0) |

(13) g (1/2,1/2,0) x,x,z (m,xyz | 1/2,1/2,0) | (14) m x+1/2,x,z (m,xyz | 1/2,1/2,0) | (15) 4* 1/2,0,z; 1/2,0,0 | (16) 4* 0,1/2,z; 0,1/2,0 |

(17) g (1/2,1/4,1/4) x,y+1/4,y (m,yz | 1/2,1/2,0) | (18) 4* x,1/4,-1/4; 1/4,1/4,-1/4 (19) 4* x,1/4,1/4; 1/4,1/4,1/4 (20) g (1/2,1/4,-1/4) x,y+1/4,y (m,yz | 1/2,1/2,0) |

(21) g (1/4,1/2,1/4) x+1/4,y,x (m,xz | 1/2,1/2,0) | (22) 4* 1/4,y,-1/4; 1/4,1/4,-1/4 (23) g (1/4,1/2,-1/4) x+1/4,y,x (m,xz | 1/2,1/2,0) | (24) 4* 1/4,y,1/4; 1/4,1/4,1/4 (m,xz | 1/2,1/2,0) |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

96 i 1

| (1) x,y,z [u,v,w] | (2) x,y,z [u,v,w] | (3) x,y,z [u,v,w] | (4) x,y,z [u,v,w] |
| (5) z,x,y [w,u,v] | (6) z,x,y [w,u,v] | (7) z,x,y [w,u,v] | (8) z,x,y [w,u,v] |
| (9) y,z,x [v,w,u] | (10) y,z,x [v,w,u] | (11) y,z,x [v,w,u] | (12) y,z,x [v,w,u] |
| (13) y,x,z [v,u,w] | (14) y,x,z [v,u,w] | (15) y,x,z [v,u,w] | (16) y,x,z [v,u,w] |
| (17) x,z,y [u,w,v] | (18) x,z,y [u,w,v] | (19) x,z,y [u,w,v] | (20) x,z,y [u,w,v] |
| (21) z,y,x [w,v,u] | (22) z,y,x [w,v,u] | (23) z,y,x [w,v,u] | (24) z,y,x [w,v,u] |

48 h ..m x,x,z [u,u,0] | x,x,z [u,u,0] | x,x,z [u,u,0] | x,x,z [u,u,0] |
Z,x,x [0,u,0] | Z,x,x [0,u,0] | Z,x,x [0,u,0] | Z,x,x [0,u,0] |
X,x,x [u,0,u] | X,x,x [u,0,u] | X,x,x [u,0,u] | X,x,x [u,0,u] |

24 g 2.mm x,1/4,1/4 [0,0,0] | x,3/4,1/4 [0,0,0] | 1/4,x,1/4 [0,0,0] |
| 1/4,x,3/4 [0,0,0] | 1/4,1/4,x [0,0,0] | 3/4,1/4,x [0,0,0] |
| 24.f | 2mm | x,0,0 [0,0,0] | x,0,0 [0,0,0] | 0,x,0 [0,0,0] |
|------|-----|----------------|
|      |     | 0,x,0 [0,0,0] | 0,0,x [0,0,0] | 0,0,0 [0,0,0] |
| 16.e | .3m | x,x,x [0,0,0] | x,x,x [0,0,0] | x,x,x [0,0,0] |
| 4.d  | 43m | 3/4,3/4,3/4 [0,0,0] |
| 4.c  | 43m | 1/4,1/4,1/4 [0,0,0] |
| 4.b  | 43m | 1/2,1/2,1/2 [0,0,0] |
| 4.a  | 43m | 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm
\[ a^* = a/2 \quad b^* = b/2 \]
Origin at 0,0,z

Along [1,1,1] p31m
\[ a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6 \]
Origin at x,x,x

Along [1,1,0] c1m11'
\[ a^* = (-a + b)/2 \quad b^* = c \]
Origin at x,x,0
Origin at $\overline{4}3m1'$

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x, 1/2-x); \quad -y \leq z \leq y \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4 \]

Symmetry Operations

For $(0,0,0) + \text{set}$

(1) $1$

(1|0,0,0)

(2) $2$ $0,0,z$

(2|0,0,0)

(3) $2$ $0,y,0$

(2|0,0,0)

(4) $2$ $x,0,0$

(2|0,0,0)

(5) $3^+$ $x,x,x$

(3_{xyz}|0,0,0)

(6) $3^+$ $x,x,x$

(3_{xyz}^{-1}|0,0,0)

(7) $3^+$ $x,x,x$

(3_{xyz}^{-1}|0,0,0)

(8) $3^+$ $x,x,x$

(3_{xyz}^{-1}|0,0,0)

(9) $3^-$ $x,x,x$

(3_{xyz}^{-1}|0,0,0)

(10) $3^-$ $x,x,x$

(3_{xyz}^{-1}|0,0,0)

(11) $3^-$ $x,x,x$

(3_{xyz}^{-1}|0,0,0)

(12) $3^-$ $x,x,x$

(3_{xyz}^{-1}|0,0,0)
For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1/2,1/2,0)

(5) 3' (1/3,1/3,1/3)
   x+1/6,x+1/3,x
   (3_{xyz}^{-1} | 1/2,1/2,0)

(9) 3' (1/3,1/3,1/3)
   x+1/3,x+1/6,x
   (3_{xyz}^{-1} | 1/2,1/2,0)

(13) g (1/2,1/2,0) x,x,z
    (m_{xy} | 1/2,1/2,0)

(17) g (1/4,1/2,1/4) x,y+1/4,y
    (m_{yz} | 1/2,1/2,0)

(21) g (1/4,1/2,1/4) x+1/4,y,x
    (m_{xz} | 1/2,1/2,0)

For (0,0,0) + set

(1) 1' (0,0,0)
(1 | 0,0,0)

(5) 3' ' x,x,x
   (3_{xyz} | 0,0,0)

(9) 3' ' x,x,x
   (3_{xyz}^{-1} | 0,0,0)

(13) m' x,x,z
    (m_{xy} | 0,0,0)

(17) m' x,y,y
    (m_{yz} | 0,0,0)

(21) m' x,y,x
    (m_{xz} | 0,0,0)

For (0,1/2,1/2) + set

(1) t' (0,1/2,1/2)
(1/0,1/2,1/2)

(5) 3' ' (1/3,1/3,1/3)
   x+1/3,x+1/6,x
   (3_{xyz}^{-1} | 1/2,1/2,2)

(9) 3' ' (1/3,1/3,1/3)
   x+1/6,x+1/6,x
   (3_{xyz}^{-1} | 0,1/2,1/2)

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Continued 216.2.1578  F4 3m1'

For (1/2,0,1/2) + set

(1) t' (1/2,0,1/2) (2) 2' (0,0,1/2) 1/4,0,0 1/4,1/4,0 1/4,1/4,1/4 1/4,1/4,1/4
(1 | 2,0,1/2)' (2 | 1/2,0,1/2)' (3 | 1/2,0,1/2)' (4 | 1/2,0,1/2)'  

(13) g' (1/4,1/4,1/2) x+1/4,x,z  
(m_xz | 1/2,0,1/2)'  

(14) g' (-1/4,1/4,1/2) 1/4,0,0 1/4,1/4,0 1/4,1/4,1/4 1/4,1/4,1/4  
(m_xz | 1/2,0,1/2)'  

(15) 4' + 1/4,1/4,0 1/4,1/4,0 1/4,1/4,1/4 1/4,1/4,1/4  
(m_xz | 1/2,0,1/2)'  

(16) 4' - 1/4,1/4,0 -1/4,1/4,0 1/4,1/4,1/4 1/4,1/4,1/4  
(m_xz | 1/2,0,1/2)'  

Generators selected  (1); t(1,0,0); t(0,0,1); t(0,1,2,1/2); t(1,2,0,1/2); (2); (3); (5); (13); 1'.
### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + (0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)' + 96</td>
<td>i 11'</td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(5) z,x,y [0,0,0]</td>
<td>(6) z,x,y [0,0,0]</td>
</tr>
<tr>
<td>(9) y,z,x [0,0,0]</td>
<td>(10) y,z,x [0,0,0]</td>
</tr>
<tr>
<td>(13) y,x,z [0,0,0]</td>
<td>(14) y,x,z [0,0,0]</td>
</tr>
<tr>
<td>(17) x,z,y [0,0,0]</td>
<td>(18) x,z,y [0,0,0]</td>
</tr>
<tr>
<td>(21) y,x,z [0,0,0]</td>
<td>(22) y,x,z [0,0,0]</td>
</tr>
</tbody>
</table>

| Symmetry of Special Projections |

#### p4mm1'

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>4d = a/2 b* = b/2</td>
<td></td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
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</tbody>
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#### p31m1'

<table>
<thead>
<tr>
<th>Along [1,1,1]</th>
<th>p31m1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>4c = (2a - b - c)/6 b* = (-a + 2b - c)/6</td>
<td></td>
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<tr>
<td>Origin at x,x,x</td>
<td></td>
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</tbody>
</table>

#### c1m11'

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>c1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>4b = a/2 b* = b/2</td>
<td></td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>

216.2.1578 - 5 - 3565
**Origin** at $\overline{4}3'm'$

**Asymmetric unit**

\[
0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{4}; \quad -\frac{1}{4} \leq z \leq \frac{1}{4}; \quad y \leq \min(x, \frac{1}{2}-x); \quad -y \leq z \leq y
\]

**Vertices**

\[
0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4} \quad \frac{1}{4},\frac{1}{4},-\frac{1}{4}
\]

**Symmetry Operations**

For $(0,0,0) + \text{set}$

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(5) & \quad 3^+ \ x,\frac{x}{2},\frac{x}{2} \\
(5) & \quad (3_{xyz})^{0,0,0} \\
(9) & \quad 3^+ \ x,\frac{x}{2},\frac{x}{2} \\
(9) & \quad (3_{xyz})^{-1,0,0,0} \\
(10) & \quad 3^+ \ x,\frac{x}{2},\frac{x}{2} \\
(10) & \quad (3_{xyz})^{0,0,0,0} \\
(11) & \quad 3^+ \ x,\frac{x}{2},\frac{x}{2} \\
(11) & \quad (3_{xyz})^{0,0,0,0} \\
(12) & \quad 3^+ \ x,\frac{x}{2},\frac{x}{2} \\
(12) & \quad (3_{xyz})^{0,0,0,0}
\end{align*}
\]
For $(1/2,1/2,0) + \text{set}$

(1) t $(1/2,1/2,0)$  
(1) $t (1/2,1/2,0)$  
(2) 2 $1/4,1/4,z$  
(2) 2 $(1/2,1/2,0)$ $1/4,y,0$  
(3) 2 $(0,1/2,0)$ $1/4,y,0$  
(4) 2 $(1/2,0,0)$ $x,1/4,o$  
(5) $3^*$ $(1/3,1/3,1/3)$  
(6) $3^*$ $x+1/2,x,x$  
(7) $3^*$ $x+1/2,x,x$  
(8) $3^*$ $(1/3,1/3,-1/3)$ $x+1/6,x+1/3,x$  
(9) $3^*$ $(1/3,1/3,1/3)$  
(10) $3^*$ $x,x+1/2,x$  
(11) $3^*$ $(1/3,1/3,-1/3)$ $x+1/3,x+1/6,x$  
(12) $3^*$ $x,x+1/2,x$  
(13) $g'(1/2,1/2,0)$ $x,x,z$  
(14) $m' x+1/2,x,z$  
(15) $4'*'' 1/2,0,z; 1/2,0,0$  
(16) $4'*' 0,1/2,z; 0,1/2,0$  
(17) $g'(1/2,1/4,1/4) x,y+1/4,y$  
(18) $4'*' x,1/4,-1/4; 1/4,1/4,-1/4$  
(19) $4'*' x,1/4,1/4; 1/4,1/4,1/4$  
(20) $g'(1/2,1/4,-1/4) x,y+1/4,y$  
(21) $g'(1/4,1/2,1/4) x+1/4,y,x$  
(22) $4'*' 1/4,y,-1/4; 1/4,1/4,-1/4$  
(23) $g'(1/4,1/2,-1/4) x+1/4,y,x$  
(24) $4'*' 1/4,y,1/4; 1/4,1/4,1/4$  

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

96  

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(0,1/2,1/2) +</th>
<th>(1/2,0,1/2) +</th>
<th>(1/2,1/2,0) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
<td>(4) x,y,z [u,v,w]</td>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) z,x,y [w,u,v]</td>
<td>(7) z,x,y [w,u,v]</td>
</tr>
</tbody>
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<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
<th>(0,0,0) +</th>
<th>(0,1/2,1/2) +</th>
<th>(1/2,0,1/2) +</th>
<th>(1/2,1/2,0) +</th>
</tr>
</thead>
<tbody>
<tr>
<td>48 h ...m' x,x,z [u,u,w]</td>
<td>(23) z,y,x [w,v,u]</td>
<td>(24) z,y,x [w,v,u]</td>
<td>(25) z,y,x [w,v,u]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24 g 2.m'm' x,1/4,1/4 [u,0,0]</td>
<td>x,3/4,1/4 [u,0,0]</td>
<td>1/4,x,1/4 [0,u,0]</td>
<td>1/4,x,3/4 [0,u,0]</td>
<td>1/4,1/4,x [0,0,u]</td>
<td>3/4,1/4,x [0,0,u]</td>
</tr>
</tbody>
</table>
24  f  $2.m'm' \  x,0,0 [u,0,0]$  \[x,0,0 [u,0,0] \quad 0,x,0 [0,u,0] \quad 0,0,0 [u,0,0] \]

16  e  $.3m' \  x,x,x [u,u,u] \ [x,x,x [u,u,u] \quad  x,x,x [u,u,u] \quad  x,x,x [u,u,u]$

4   d  $\bar{4}3m' \  3/4,3/4,3/4 [0,0,0]$

4   c  $\bar{4}3m' \  1/4,1/4,1/4 [0,0,0]$

4   b  $\bar{4}3m' \  1/2,1/2,1/2 [0,0,0]$

4   a  $\bar{4}3m' \  0,0,0 [0,0,0]$

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along</th>
<th>$[0,0,1]$</th>
<th>$[1,1,1]$</th>
<th>$[1,1,0]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^*$</td>
<td>$a/2$</td>
<td>$(2a - b - c)/6$</td>
<td>$(-a + b)/2$</td>
</tr>
<tr>
<td>$b^*$</td>
<td>$b/2$</td>
<td>$(-a + 2b - c)/6$</td>
<td>$c$</td>
</tr>
</tbody>
</table>

Origin at $0,0,z$  
Origin at $x,x,x$  
Origin at $x,x,0$
Origin at \( \bar{4}3m \)

Asymmetric unit: 
\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y \]

Vertices: 
\[ 0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2 \]

Symmetry Operations:

For \((0,0,0)\) + set

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 2 \quad 0,y,0
\\
(4) & \quad 2 \quad x,0,0
\\
(5) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz} \quad 0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1} \quad 0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1} \quad 0,0,0) \\
(8) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz}^{-1} \quad 0,0,0) \\
(9) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1} \quad 0,0,0) \\
(10) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz} \quad 0,0,0) \\
(11) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz} \quad 0,0,0) \\
(12) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz} \quad 0,0,0)
\end{align*}
Continued

(13) m x,x,z  
(m_{xy} | 0,0,0)  
(14) m x,x,z  
(m_{xy} | 0,0,0)  
(15) 4^+ 0,0,z; 0,0,0  
(4_z | 0,0,0)  
(16) 4^- 0,0,z; 0,0,0  
(4_z^- | 0,0,0)  
(17) m x,y,y  
(m_{yz} | 0,0,0)  
(18) 4^- x,0,0; 0,0,0  
(4_x^- | 0,0,0)  
(19) 4^- x,0,0; 0,0,0  
(4_x^- | 0,0,0)  
(20) m x,y,y  
(m_{yz} | 0,0,0)  
(21) m x,y,x  
(m_{xz} | 0,0,0)  
(22) 4^- 0,y,0; 0,0,0  
(4_y^- | 0,0,0)  
(23) m x,y,x  
(m_{xz} | 0,0,0)  
(24) 4^+ 0,y,0; 0,0,0  
(4_y^+ | 0,0,0)  

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)  
(2) 2 (0,0,1/2) 1/4,1/4,z  
(2_z | 1/2,1/2,1/2)  
(3) 2 (0,1/2,0) 1/4,y,1/4  
(2_y | 1/2,1/2,1/2)  
(4) 2 (1/2,0,0) x,1/4,1/4  
(2_x | 1/2,1/2,1/2)  
(5) 3^- (1/2,1/2,1/2) x,x,x  
(3_{xyz} | 1/2,1/2,1/2)  
(6) 3^- (1/6,-1/6,1/6) x+1/3,x+1/3,x+1/3  
(3_{xyz}^- | 1/2,1/2,1/2)  
(7) 3^- (-1/6,1/6,1/6) x+2/3,x-1/3,x  
(3_{xyz}^- | 1/2,1/2,1/2)  
(8) 3^- (1/6,1/6,-1/6) x+1/3,x+2/3,x  
(3_{xyz}^- | 1/2,1/2,1/2)  
(9) 3^- (1/2,1/2,1/2) x,x,x  
(3_{xyz}^- | 1/2,1/2,1/2)  
(10) 3^- (-1/6,1/6,1/6) x+1/3,x+1/3,x+1/3  
(3_{xyz}^- | 1/2,1/2,1/2)  
(11) 3^- (1/6,1/6,-1/6) x+2/3,x+1/3,x  
(3_{xyz}^- | 1/2,1/2,1/2)  
(12) 3^- (1/6,-1/6,1/6) x-1/3,x+2/3,x  
(3_{xyz}^- | 1/2,1/2,1/2)  
(13) n (1/2,1/2,1/2) x,x,z  
(m_{xy} | 1/2,1/2,1/2)  
(14) c (0,0,1/2) x+1/2,x+1/2,z  
(m_{xy} | 1/2,1/2,1/2)  
(15) 4^+ 1/2,0,z; 1/2,0,1/4  
(4_z | 1/2,1/2,1/2)  
(16) 4^- 0,1/2,z; 0,1/2,1/4  
(4_z^- | 1/2,1/2,1/2)  
(17) n (1/2,1/2,1/2) x,y,y  
(m_{yz} | 1/2,1/2,1/2)  
(18) 4^- x,1/2,0;1/4,1/2,0  
(4_x^- | 1/2,1/2,1/2)  
(19) 4^- x,0,1/2;1/4,0,1/2  
(4_x^- | 1/2,1/2,1/2)  
(20) a (1/2,0,0) x,y+1/2,y  
(m_{yz} | 1/2,1/2,1/2)  
(21) n (1/2,1/2,1/2) x,y,x  
(m_{xz} | 1/2,1/2,1/2)  
(22) 4^- 1/2,y,0; 1/2,1/4,0  
(4_y^- | 1/2,1/2,1/2)  
(23) b (0,1/2,0) x+1/2,y,x  
(m_{xz} | 1/2,1/2,1/2)  
(24) 4^+ 0,y,1/2; 0,1/4,1/2  
(4_y^+ | 1/2,1/2,1/2)  

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

48  

h  

1  

(1) x,y,z [u,v,w]  
(2) z,x,y [u,v,w]  
(3) x,y,z [u,v,w]  
(4) x,y,z [u,v,w]  
(5) z,x,y [w,u,v]  
(6) z,x,y [w,u,v]  
(7) z,x,y [w,u,v]  
(8) z,x,y [w,u,v]  
(9) y,z,x [v,w,u]  
(10) y,z,x [v,w,u]  
(11) y,z,x [v,w,u]  
(12) y,z,x [v,w,u]  
(13) y,z,x [v,w,u]  
(14) y,z,x [v,w,u]  
(15) y,z,x [v,w,u]  
(16) y,z,x [v,w,u]  
(17) x,z,y [u,w,v]  
(18) x,z,y [u,w,v]  
(19) x,z,y [u,w,v]  
(20) x,z,y [u,w,v]  
(21) z,y,x [w,v,u]  
(22) z,y,x [w,v,u]  
(23) z,y,x [w,v,u]  
(24) z,y,x [w,v,u]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>24</th>
<th>g</th>
<th>24</th>
<th>f</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>g</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>g</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Origin at 0,0,z**

<table>
<thead>
<tr>
<th>12</th>
<th>e</th>
<th>12</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>e</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>d</td>
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<td></td>
</tr>
</tbody>
</table>

**Origin at x,x,x**

<table>
<thead>
<tr>
<th>8</th>
<th>c</th>
<th>6</th>
<th>b</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>c</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Origin at x,x,0**

<table>
<thead>
<tr>
<th>2</th>
<th>a</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>a</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4'mmm'</th>
<th>Along [1,1,1]</th>
<th>p31m</th>
<th>Along [1,1,0]</th>
<th>p1m11'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (a - b)/2</td>
<td>b* = (a + b)/2</td>
<td>a* = (2a - b - c)/3</td>
<td>b* = (-a + 2b - c)/3</td>
<td>a* = (-a + b)/2</td>
<td>b* = c/2</td>
</tr>
</tbody>
</table>

**Origin at 0,0,z**

| 217.1.1580 - 3 - 3572 |
Origin at \( \overline{4}3m1' \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y \]

Vertices

\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 1/2,1/2,1/2
\end{align*}

Symmetry Operations

For \((0,0,0) + \text{set}\)

\begin{align*}
(1) & \quad 1 & \quad \text{For \((0,0,0) + \text{set}\)} \\
(1) & \quad 0,0,z & \quad (2) & \quad 0,y,0 & \quad (3) & \quad 0,z,0 & \quad (4) & \quad x,0,0 & \quad (2,0,0,0) \\
(5) & \quad 3^+ x,x,x & \quad (2) & \quad 3^+ x,y,x & \quad (2) & \quad x,0,0 & \quad (2,0,0,0) \\
(3) & \quad 0,0,0 & \quad (3) & \quad y,0,0 & \quad (3) & \quad y,0,0 & \quad (3) & \quad y,0,0 \\
(9) & \quad x,x,x & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0 \\
(10) & \quad x,x,x & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0 \\
(11) & \quad x,x,x & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0 \\
(12) & \quad x,x,x & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0 & \quad (3) & \quad x,x,0
\end{align*}
For \((1/2,1/2,1/2)' + \text{set}\)

(1) \(t'\ (1/2,1/2,1/2)\)
(2) \(2'\ (0,0,1/2)\)
(3) \(2'\ (0,1/2,0)\)
(4) \(2'\ (1/2,0,0)\)
(5) \(3'\ (1/2,1/2,1/2)\)
(6) \(3'\ (1/6,-1/6,1/6)\)
(7) \(3'\ (-1/6,1/6,1/6)\)
(8) \(3'\ (1/6,1/6,-1/6)\)
(9) \(3'\ (1/2,1/2,1/2)\)
(10) \(3'\ (-1/6,1/6,-1/6)\)
(11) \(3'\ (1/6,-1/6,1/6)\)
(12) \(3'\ (1/6,1/6,-1/6)\)
(13) \(n'\ (1/2,1/2,1/2)\)
(14) \(c'\ (0,0,1/2)\)
(15) \(4\ (1/2,0,0)\)
(16) \(4\ (1/2,1/2,1/2)\)
(17) \(n'\ (1/2,1/2,1/2)\)
(18) \(4\ (1/2,1/2,1/2)\)
(19) \(4\ (1/2,1/2,1/2)\)
(20) \(4\ (1/2,1/2,1/2)\)
(21) \(n'\ (1/2,1/2,1/2)\)
(22) \(4\ (1/2,1/2,1/2)\)
(23) \(4\ (1/2,1/2,1/2)\)
(24) \(4\ (1/2,1/2,1/2)\)

Generators selected

(1); \(t(1,0,0)\); \(t(0,1,0)\); \(t(0,0,1)\); \(t(1/2,1/2,1/2)\); (2); (3); (5); (13); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Generator</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0)) + ((1/2,1/2,1/2)) + ((0,0,0)' + (1/2,1/2,1/2))' +</td>
<td></td>
</tr>
</tbody>
</table>
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Projection</th>
<th>Axes</th>
<th>Formula for (a^*)</th>
<th>Formula for (b^*)</th>
<th>Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>p4mm1'</td>
<td>[0,0,1]</td>
<td>(a^* = \frac{a - b}{2})</td>
<td>(b^* = \frac{a + b}{2})</td>
<td>0,0,z</td>
</tr>
<tr>
<td>p31m1'</td>
<td>[1,1,1]</td>
<td>(a^* = \frac{2a - b - c}{3})</td>
<td>(b^* = \frac{-a + 2b - c}{3})</td>
<td>x,x,x</td>
</tr>
<tr>
<td>p1m11'</td>
<td>[1,1,0]</td>
<td>(a^* = \frac{a + b}{2})</td>
<td>(b^* = \frac{c}{2})</td>
<td>x,x,0</td>
</tr>
</tbody>
</table>
Origin at \( \bar{4}3m' \)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y \]

Vertices

\[ 0,0,0 \quad \text{and} \quad 1/2,0,0 \quad \text{and} \quad 1/2,1/2,0 \quad \text{and} \quad 1/2,1/2,1/2 \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. 1
   \((1|0,0,0)\)
2. 2 0,0,z
   \((2|0,0,0)\)
3. 2 0,y,0
   \((2|0,0,0)\)
4. 2 x,0,0
   \((2|0,0,0)\)
5. \(3^+ x,x,x\)
   \((3_{xyz}|0,0,0)\)
6. \(3^+ x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)
7. \(3^+ x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)
8. \(3^+ x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)
9. \(3^- x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)
10. \(3^- x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)
11. \(3^- x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)
12. \(3^- x,x,x\)
   \((3_{xyz}^{-1}|0,0,0)\)
Continued

217.2.1581  I43m1

(13) m'  x,x,z
       (m_xz|0,0,0)'
(14) m'  x,x,z
       (m_xy|0,0,0)'
(15) 4''  0,0,z; 0,0,0
       (4_z|0,0,0)'
(16) 4''  0,0,z; 0,0,0
       (4_z|0,0,0)'
(17) m'  x,y,y
       (m_yz|0,0,0)'
(18) 4''  x,0,0; 0,0,0
       (4_y,0,0,0)'
(19) 4''  x,0,0; 0,0,0
       (4_y,0,0,0)'
(20) m'  x,y,y
       (m_yz|0,0,0)'
(21) m'  x,y,x
       (m_xz|0,0,0)'
(22) 4''  0,y,0; 0,0,0
       (4_y,0,0,0)'
(23) m'  x,y,x
       (m_xz|0,0,0)'
(24) 4''  0,y,0; 0,0,0
       (4_y,0,0,0)'

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(2) 2 (0,0,1/2) 1/4,1/4,z
(2|z|1/2,1/2,1/2)
(3) 2 (0,1/2,0) 1/4,y,1/4
(2|y|1/2,1/2,1/2)
(4) 2 (1/2,0,0) x,1/4,1/4
(2|x|1/2,1/2,1/2)
(5) 3' (1/2,1/2,1/2) x,x,x
(3_xz|1/2,1/2,1/2)
(6) 3' (1/6,-1/6,1/6)
(3_xz-1|1/2,1/2,1/2)
(7) 3' (-1/6,1/6,1/6)
(3_xz-1|1/2,1/2,1/2)
(8) 3' (1/6,1/6,-1/6)
(3_xz-1|1/2,1/2,1/2)
(9) 3' (1/2,1/2,1/2) x,x,x
(3_xz-1|1/2,1/2,1/2)
(10) 3' (-1/6,1/6,1/6)
(3_xz-1|1/2,1/2,1/2)
(11) 3' (1/6,1/6,-1/6)
(3_xz-1|1/2,1/2,1/2)
(12) 3' (1/6,1/6,-1/6)
(3_xz-1|1/2,1/2,1/2)
(13) n' (1/2,1/2,1/2) x,x,z
       (m_xy|1/2,1/2,1/2)'
(14) c' (0,0,1/2)
       (m_xy|1/2,1/2,1/2)'
(15) 4''  1/2,0,z; 1/2,0,1/4
       (4_z|1/2,1/2,1/2)'
(16) 4''  1/2,0,z; 0,1/2,1/4
       (4_z|1/2,1/2,1/2)'
(17) n' (1/2,1/2,1/2) x,y,y
       (m_yz|1/2,1/2,1/2)'
(18) 4''  x,1/2,0; 1/4,1/2,0
       (4_x|1/2,1/2,1/2)'
(19) 4''  x,0,1/2; 1/4,0,1/2
       (4_x|1/2,1/2,1/2)'
(20) a' (1/2,0,0) x,y+1/2,1/2
       (m_yz|1/2,1/2,1/2)'
(21) n' (1/2,1/2,1/2) x,y,x
       (m_xz|1/2,1/2,1/2)'
(22) 4''  1/2,0,y; 1,2,1/4,0
       (4_y,1/2,1/2,1/2)'
(23) b' (0,1/2,0)
       (m_xz|1/2,1/2,1/2)'
(24) 4''  0,y,1/2; 0,1,4,1/2
       (4_y,1/2,1/2,1/2)'

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

(0,0,0) +
(1/2,1/2,1/2) +

48  h  1

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) x,y,z [u,v,w]
(4) x,y,z [u,v,w]
(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]
(9) y,z,x [v,w,u]
(10) y,z,x [v,w,u]
(11) y,z,x [v,w,u]
(12) y,z,x [v,w,u]
(13) y,x,z [v,u,w]
(14) y,x,z [v,u,w]
(15) y,x,z [v,u,w]
(16) y,x,z [v,u,w]
(17) x,z,y [u,w,v]
(18) x,z,y [u,w,v]
(19) x,z,y [u,w,v]
(20) x,z,y [u,w,v]
(21) z,y,x [w,v,u]
(22) z,y,x [w,v,u]
(23) z,y,x [w,v,u]
(24) z,y,x [w,v,u]

217.3.1582 - 2 - 3578
Continued

217.3.1581
I 4 3m1'

24 g  ..m'  x,x,z [u,u,w]  x,x,z [u,u,w]  x,x,z [u,u,w]  
    z,x,x [w,u,u]  z,x,x [w,u,u]  z,x,x [w,u,u]  
    x,z,x [u,w,u]  x,z,x [u,w,u]  x,z,x [u,w,u]  

24 f  2..  x,1/2,0 [u,0,0]  x,1/2,0 [u,0,0]  0,x,1/2 [0,u,0]  0,x,1/2 [0,u,0]  
    1/2,0,x [0,0,u]  1/2,0,x [0,0,u]  1/2,x,0 [0,u,0]  1/2,x,0 [0,u,0]  
    x,0,1/2 [u,0,0]  x,0,1/2 [u,0,0]  0,1/2,x [0,0,u]  0,1/2,x [0,0,u]  

12 e  2.m'm'  x,0,0 [u,0,0]  x,0,0 [u,0,0]  0,x,0 [0,u,0]  0,x,0 [0,u,0]  
    0,0,x [0,0,u]  0,0,x [0,0,u]  0,0,x [0,0,u]  0,0,x [0,0,u]  

12 d  4'  1/4,1/2,0 [0,0,0]  3/4,1/2,0 [0,0,0]  0,1/4,1/2 [0,0,0]  0,1/4,1/2 [0,0,0]  
    0,3/4,1/2 [0,0,0]  1/2,0,1/4 [0,0,0]  1/2,0,1/4 [0,0,0]  1/2,0,3/4 [0,0,0]  

8 c  .3m'  x,x,x [u,u,u]  x,x,x [u,u,u]  x,x,x [u,u,u]  x,x,x [u,u,u]  

6 b  4'2.m'  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,1,2/0 [0,0,0]  

2 a  4'3m'  0,0,0 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1]  p4m'm'  
A* = (a - b)/2  B* = (a + b)/2  
Origin at 0,0,0

Along [1,1,1]  p31m'  
A* = (2a - b - c)/3  B* = (-a + 2b - c)/3  
Origin at x,x,x

Along [1,1,0]  p1m'  
A* = (a + b)/2  B* = c/2  
Origin at x,x,0
Origin at \(\overline{43m}\)

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y
\]

Vertices

\[
0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2
\]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{align*}
(1) & \quad \mathbf{1} \\
(1) & \quad (0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
(2) & \quad (0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
(3) & \quad (0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
(4) & \quad (0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
(5) & \quad (0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
(6) & \quad (0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
(7) & \quad (0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
(8) & \quad (0,0,0) \\
(9) & \quad 3^- \quad x,x,x \\
(9) & \quad (0,0,0) \\
(10) & \quad 3^- \quad x,x,x \\
(10) & \quad (0,0,0) \\
(11) & \quad 3^- \quad x,x,x \\
(11) & \quad (0,0,0) \\
(12) & \quad 3^- \quad x,x,x \\
(12) & \quad (0,0,0)
\end{align*}
\]
Continued

$$\begin{align*}
(13) \ m \ x,x,z \\
& (m_{xy}|0,0,0) \\
(14) \ m \ x,x,z \\
& (m_{xy}|0,0,0) \\
(15) \ 4^+ \ 0,0,z; 0,0,0 \\
& (4^-|0,0,0) \\
(16) \ 4^- \ 0,0,z; 0,0,0 \\
& (4^-|0,0,0) \\
(17) \ m \ x,y,y \\
& (m_{yz}|0,0,0) \\
(18) \ 4^+ \ x,0,0; 0,0,0 \\
& (4^-|0,0,0) \\
(19) \ 4^- \ x,0,0; 0,0,0 \\
& (4^-|0,0,0) \\
(20) \ m \ x,y,$$

$$\begin{align*}
(21) \ m \ x,y,x \\
& (m_{zx}|0,0,0) \\
(22) \ 4^- \ 0,y,0; 0,0,0 \\
& (4^-|0,0,0) \\
(23) \ m \ x,y,x \\
& (m_{zx}|0,0,0) \\
(24) \ 4^- \ 0,y,0; 0,0,0 \\
& (4^-|0,0,0)
\end{align*}
$$

For (1/2,1/2,1/2) + set

$$\begin{align*}
(1) \ t' \ (1/2,1/2,1/2) \\
& (1|1/2,1/2,1/2)' \\
(2) \ 2' \ (0,0,1/2) \ 1/4,1/4,z \\
& (2|1/2,1/2,1/2)' \\
(3) \ 2' \ (0,1/2,0) \ 1/4,y,1/4 \\
& (2|1/2,1/2,1/2)' \\
(4) \ 2' \ (1/2,0,0) \ x,1/4,1/4 \\
& (2|1/2,1/2,1/2)' \\
(5) \ 3' \ (1/2,1/2,1/2) \ x,x,x \\
& (3_{xy}|1/2,1/2,1/2)' \\
(6) \ 3' \ (1/6,1/6,1/6) \ \overline{x}+1/3,\overline{x}+1/3,\overline{x} \\
& (3_{xy}|1/2,1/2,1/2)' \\
(7) \ 3' \ (-1/6,1/6,1/6) \ x+2/3,x-1/3,x \\
& (3_{xy}|1/2,1/2,1/2)' \\
(8) \ 3' \ (1/6,1/6,-1/6) \ x+1/3,x+2/3,x \\
& (3_{xy}|1/2,1/2,1/2)' \\
(9) \ 3' \ (1/2,1/2,1/2) \ x,x,x \\
& (3_{xy}|1/2,1/2,1/2)' \\
(10) \ 3' \ (-1/6,1/6,1/6) \ \overline{x}+1/3,\overline{x}+1/3,\overline{x} \\
& (3_{xy}|1/2,1/2,1/2)' \\
(11) \ 3' \ (1/6,1/6,-1/6) \ x+2/3,x+1/3,x \\
& (3_{xy}|1/2,1/2,1/2)' \\
(12) \ 3' \ (1/6,1/6,1/6) \ x-1/3,x+2/3,x \\
& (3_{xy}|1/2,1/2,1/2)' \\
(13) \ n' \ (1/2,1/2,1/2) \ x,x,z \\
& (m_{xy}|1/2,1/2,1/2)' \\
(14) \ n' \ (1/2,1/2,1/2) \ \overline{x}+1/2,\overline{x},z \\
& (m_{xy}|1/2,1/2,1/2)' \\
(15) \ 4^+ \ (1/2,0,0; 1/2,0,1/4 \\
& (4^-|1/2,1/2,1/2)' \\
(16) \ 4^- \ 0,1/2,z; 0,1/2,1/4 \\
& (4^-|1/2,1/2,1/2)' \\
(17) \ n' \ (1/2,1/2,1/2) \ x,y,y \\
& (m_{yz}|1/2,1/2,1/2)' \\
(18) \ n' \ (1/2,1/2,1/2) \ x,1/2,0; 1/4,1/2,0 \\
& (4^-|1/2,1/2,1/2)' \\
(19) \ 4^- \ x,0,1/2; 1/4,0,1/2 \\
& (4^-|1/2,1/2,1/2)' \\
(20) \ a' \ (1/2,0,0) \ x,y+1/2,\overline{y} \\
& (m_{yz}|1/2,1/2,1/2)' \\
(21) \ n' \ (1/2,1/2,1/2) \ x,y,x \\
& (m_{zx}|1/2,1/2,1/2)' \\
(22) \ n' \ (1/2,1/2,1/2) \ \overline{y}+1/2,\overline{y},x \\
& (m_{zx}|1/2,1/2,1/2)' \\
(23) \ b' \ (0,1/2,0) \ \overline{x}+1/2,\overline{y},x \\
& (m_{zx}|1/2,1/2,1/2)' \\
(24) \ 4^+ \ 0,y,1/2; 0,1/4,1/2 \\
& (4^-|1/2,1/2,1/2) \\
& (4^-|1/2,1/2,1/2) \\
& (4^-|1/2,1/2,1/2) \\
& (4^-|1/2,1/2,1/2)
\end{align*}
$$

Generators selected

$$\begin{align*}
(1) \ t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13).
\end{align*}$$

Positions

- Multicplicity
- Wyckoff letter
- Site Symmetry

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$$\begin{align*}
(1) \ x,y,z [u,v,w] \\
& (2) \ x,\overline{y},z [\overline{u},\overline{v},w] \\
& (3) \ x,y,\overline{z} [u,v,\overline{w}] \\
& (4) \ x,y,\overline{z} [u,\overline{v},w] \\
(5) \ z,x,y [w,u,v] \\
& (6) \ z,\overline{x},\overline{y} [w,\overline{u},\overline{v}] \\
& (7) \ \overline{z},x,\overline{y} [\overline{w},u,v] \\
& (8) \ \overline{z},x,\overline{y} [\overline{w},u,\overline{v}] \\
(9) \ y,z,x [v,w,u] \\
& (10) \ y,\overline{z},\overline{x} [\overline{v},w,\overline{u}] \\
& (11) \ y,\overline{z},\overline{x} [v,\overline{w},u] \\
& (12) \ y,\overline{z},\overline{x} [v,\overline{w},\overline{u}] \\
(13) \ y,z,x [\overline{v},u,\overline{w}] \\
& (14) \ y,\overline{z},\overline{x} [v,\overline{w},u] \\
& (15) \ y,\overline{z},\overline{x} [v,\overline{w},\overline{u}] \\
& (16) \ y,\overline{z},\overline{x} [\overline{v},u,\overline{w}] \\
(17) \ x,z,y [u,w,v] \\
& (18) \ x,\overline{z},\overline{y} [u,\overline{w},v] \\
& (19) \ x,z,\overline{y} [u,w,\overline{v}] \\
& (20) x,z,y [u,w,v] \\
(21) \ z,y,x [\overline{w},v,\overline{u}] \\
& (22) z,\overline{y},\overline{x} [\overline{w},v,\overline{u}] \\
& (23) z,\overline{y},\overline{x} [\overline{w},v,u] \\
& (24) \overline{z},\overline{y},x [\overline{w},v,\overline{u}]
\end{align*}$$

217.4.1583 - 2 - 3581
Symmetry of Special Projections

Along \([0,0,1]\) \(p_4\) 4m\(m'\)  
\(a^* = (a - b)/2\)  \(b^* = (a + b)/2\)  
Origin at 1/2,0,z

Along \([1,1,1]\) \(p31m\) 1'  
\(a^* = (2a - b - c)/3\)  \(b^* = (-a + 2b - c)/3\)  
Origin at x,x,x

Along \([1,1,0]\) \(p1m1\) 1'  
\(a^* = (-a + b)/2\)  \(b^* = c/2\)  
Origin at x,x,0
Origin at $4'3m'$

Asymmetric unit

\[ 0 \leq x < 1/2; \quad 0 \leq y < 1/2; \quad 0 \leq z < 1/2; \quad y < x; \quad z < y \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2 \]

Symmetry Operations

For \((0,0,0) + \text{set}\)

(1) \(1\)
(2) \(2\) \(0,0,z\)
(3) \(2\) \(0,y,0\)
(4) \(2\) \(x,0,0\)
(5) \(3^+\) \(x,x,x\)
(6) \(3^+\) \(x,x,x\)
(7) \(3^+\) \(x,x,x\)
(8) \(3^+\) \(x,x,x\)
(9) \(3^-\) \(x,x,x\)
(10) \(3^-\) \(x,x,x\)
(11) \(3^-\) \(x,x,x\)
(12) \(3^-\) \(x,x,x\)

\(3xyz|0,0,0\)

\(3xyz|0,0,0\)

\(3xyz^{-1}|0,0,0\)

\(3xyz^{-1}|0,0,0\)
Continued

217.5.1584

(13) $m' \times x, x, z$

(14) $m' \times x, x, z$

(15) $4^{+}\cdot 0, 0, z; 0, 0, 0$

(16) $4^{+}\cdot 0, 0, z; 0, 0, 0$

(17) $m' \times y, y$

(18) $4^{+}\cdot 0, 0, 0; 0, 0, 0$

(19) $4^{+}\cdot x, 0, 0; 0, 0, 0$

(20) $m' \times y, y$

(21) $m' \times y, x$

(22) $4^{+}\cdot 0, y, 0; 0, 0, 0$

(23) $m' \times y, y$

(24) $4^{+}\cdot 0, y, 0; 0, 0, 0$

For $(1/2, 1/2, 1/2)^{\prime} +$ set

(1) $t' (1/2, 1/2, 1/2)^{\prime}$

(2) $2' (0, 1/2, 0) 1/4, 1/4, z$

(3) $2' (0, 1/2, 0) 1/4, 1/4, z$

(4) $2' (1/2, 0, 0) x, 1/4, 1/4$

(5) $3^{+}\cdot (1/2, 1/2, 1/2) x, x, x$

(6) $3^{+}\cdot (1/6, -1/6, 1/6) x + 1/3, x + 1/3, x$

(7) $3^{+}\cdot (1/6, 1/6, -1/6) x + 1/3, x - 1/3, x$

(8) $3^{+}\cdot (1/6, 1/6, -1/6) x + 1/3, x + 2/3, x$

(9) $3^{+}\cdot (1/2, 1/2, 1/2) x, x, x$

(10) $3^{+}\cdot (-1/6, 1/6, 1/6) x + 1/3, x + 1/3, x$

(11) $3^{+}\cdot (-1/6, 1/6, -1/6) x + 1/3, x + 2/3, x$

(12) $3^{+}\cdot (1/2, 1/2, 1/2) x, x, x$

(13) $n (1/2, 1/2, 1/2) x, x, z$

(14) $c (0, 1/2, 0) x + 1/2, x, z$

(15) $4^{+} 1/2, 0, z; 1/2, 0, 1/4$

(16) $4^{+} 0, 1/2, z; 0, 1/2, 1/4$

(17) $n (1/2, 1/2, 1/2) x, y, y$

(18) $4^{+} x, 1/2, 0; 1/4, 1/2, 0$

(19) $4^{+} x, 0, 1/2; 1/4, 0, 1/2$

(20) $a (1/2, 0, 0) x, y + 1/2, y$

(21) $n (1/2, 1/2, 1/2) x, y, x$

(22) $4^{+} 1/2, y, 0; 1/2, 1/4, 0$

(23) $b (0, 1/2, 0) x + 1/2, y, x$

(24) $4^{+} 0, y, 1/2; 0, 1/4, 1/2$

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t’(1/2,1/2,1/2); (2); (3); (5); (13).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48 h 1

(1) x,y,z [u,v,w]

(2) $x, y, z [u, v, w]$

(3) $x, y, z [u, v, w]$

(4) $x, y, z [u, v, w]$

(5) z,x,y [w,u,v]

(6) z,x,y [w,u,v]

(7) $z, x, y [w, u, v]$

(8) $z, x, y [w, u, v]$

(9) y,z,x [v,w,u]

(10) $y, z, x [v, w, u]$

(11) $y, z, x [v, w, u]$

(12) $y, z, x [v, w, u]$

(13) y,x,z [v,u,w]

(14) $y, x, z [v, u, w]$

(15) $y, x, z [v, u, w]$

(16) $y, x, z [v, u, w]$

(17) x,z,y [u,w,v]

(18) x,z,y [u,w,v]

(19) x,z,y [u,w,v]

(20) x,z,y [u,w,v]

(21) z,y,x [w,v,u]

(22) z,y,x [w,v,u]

(23) $z, y, x [w, v, u]$

(24) $z, y, x [w, v, u]$
<table>
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<tr>
<th>24 g</th>
<th>m'</th>
<th>x,x,z [u,u,w]</th>
<th>x,x,z [u,u,w]</th>
<th>x,x,z [u,u,w]</th>
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<td>z,x,x [w,u,u]</td>
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<td>x,z,x [u,w,u]</td>
</tr>
</tbody>
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<tr>
<th>24 f</th>
<th>2..</th>
<th>x,1/2,0 [u,0,0]</th>
<th>0,x,1/2 [0,u,0]</th>
<th>0,x,1/2 [0,u,0]</th>
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<td>1/2,0,x [0,0,u]</td>
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<td>0,1/2,x [0,0,u]</td>
<td>0,1/2,x [0,0,u]</td>
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</tbody>
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<tr>
<th>12 e</th>
<th>2.m'm'</th>
<th>x,0,0 [u,0,0]</th>
<th>0,x,0 [0,u,0]</th>
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<td>0,0,x [0,0,u]</td>
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<tr>
<th>12 d</th>
<th>4</th>
<th>1/4,1/2,0 [u,0,0]</th>
<th>3/4,1/2,0 [u,0,0]</th>
<th>0,1/4,1/2 [0,u,0]</th>
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<td>0,3/4,1/2 [0,u,0]</td>
<td>1/2,0,1/4 [0,0,u]</td>
<td>1/2,0,3/4 [0,0,u]</td>
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<tr>
<th>8 c</th>
<th>.3m'</th>
<th>x,x,x [u,u,u]</th>
<th>x,x,x [u,u,u]</th>
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<tr>
<th>6 b</th>
<th>4'2.m'</th>
<th>0,1/2,1/2 [0,0,0]</th>
<th>1/2,0,1/2 [0,0,0]</th>
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<th>2 a</th>
<th>4'3m'</th>
<th>0,0,0 [0,0,0]</th>
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<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**: $p_{p^*} 4m'm'$
  - $a^* = (a - b)/2$
  - $b^* = (a + b)/2$
  - Origin at 0,0,0

- **Along [1,1,1]**: $p31m1'$
  - $a^* = (2a - b - c)/3$
  - $b^* = (-a + 2b - c)/3$
  - Origin at x,x,x

- **Along [1,1,0]**: $p_{2b1}1m1$
  - $a^* = (-a + b)/2$
  - $b^* = c/2$
  - Origin at x,x,0
Origin at 23

Asymmetric unit 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; z ≤ min(x, y)

Vertices 0,0,0 1/2,0,0 1/2,1/2,0 0,1/2,0 1/2,1/2,1/2

Symmetry Operations

(1) 1
    (1|0,0,0)

(2) 2 0,0,z
    (2|0,0,0)

(3) 2 0,y,0
    (2|0,0,0)

(4) 2 x,0,0
    (2|0,0,0)

(5) 3⁺ x,x,x
    (3xyz|0,0,0)

(6) 3⁺ x,x,x
    (3xyz⁻¹|0,0,0)

(7) 3⁺ x,x,x
    (3xyz⁻¹|0,0,0)

(8) 3⁺ x,x,x
    (3xyz⁻¹|0,0,0)

(9) 3ˊ x,x,x
    (3',yz⁻¹|0,0,0)

(10) 3ˊ x,x,x
    (3',yz⁻¹|0,0,0)

(11) 3ˊ x,x,x
    (3',yz⁻¹|0,0,0)

(12) 3ˊ x,x,x
    (3',yz⁻¹|0,0,0)
Continued

Generators selected

(13) n (1/2,1/2,1/2) x,x,z
(m_x \parallel 1/2,1/2,1/2)

(14) c (0,0,1/2) x+1/2,x,x
(m_y \parallel 1/2,1/2,1/2)

(15) \( n^{4+} \) 1/2,0,z;1/2,0,1/4
(4_z \parallel 1/2,1/2,1/2)

(16) \( n^{-} \) 0,1/2,z; 0,1/2,1/4
(4_z^{-1} \parallel 1/2,1/2,1/2)

(17) n (1/2,1/2,1/2) x,y,y
(m_y \parallel 1/2,1/2,1/2)

(18) \( n^{4+} \) x,1/2,0;1/4,1/2,0
(4_x \parallel 1/2,1/2,1/2)

(19) \( n^{-} \) x,0,1/2;1/4,0,1/2
(4_x^{-1} \parallel 1/2,1/2,1/2)

(20) a (1/2,0,0) y+1/2,y
(4_y \parallel 1/2,1/2,1/2)

(21) n (1/2,1/2,1/2) x,y,x
(m_z \parallel 1/2,1/2,1/2)

(22) \( n^{4-} \) 1/2,1/2,1/2
(4_y \parallel 1/2,1/2,1/2)

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
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<tbody>
<tr>
<td>24 i 1</td>
<td>(1) x,y,z [u,v,w]</td>
</tr>
<tr>
<td></td>
<td>(2) x,y,z [u,v,w]</td>
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<td>(3) x,y,z [u,v,w]</td>
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<td>(4) x,y,z [u,v,w]</td>
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<td>(5) z,x,y [w,u,v]</td>
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<td>(6) z,x,y [w,u,v]</td>
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<td>(7) z,x,y [w,u,v]</td>
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<td>(8) z,x,y [w,u,v]</td>
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<td>(9) y,z,x [v,w,u]</td>
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<td>(10) y,z,x [v,w,u]</td>
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<td>(11) y,z,x [v,w,u]</td>
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<td>(12) y,z,x [v,w,u]</td>
</tr>
<tr>
<td></td>
<td>(13) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<tr>
<td></td>
<td>(14) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(15) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
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<td>(17) x+1/2,z+1/2,y+1/2 [w,v,u]</td>
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<td>(18) x+1/2,z+1/2,y+1/2 [w,v,u]</td>
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<td>(19) x+1/2,z+1/2,y+1/2 [w,v,u]</td>
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<tr>
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<td>(20) x+1/2,z+1/2,y+1/2 [w,v,u]</td>
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<td>(21) z+1/2,y+1/2,x+1/2 [w,v,u]</td>
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<td>(22) z+1/2,y+1/2,x+1/2 [w,v,u]</td>
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<td></td>
<td>(23) z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
<tr>
<td></td>
<td>(24) z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
</tbody>
</table>

12 h 2.. x,0,1/2 [u,0,0] x,0,1/2 [u,0,0] 1/2,x,0 [0,u,0] 1/2,x,0 [0,u,0]

0,1/2,x [0,0,u] 0,1/2,x [0,0,u] 1/2,x+1/2,0 [0,u,0] 1/2,x+1/2,0 [0,u,0]

x+1/2,0,1/2 [u,0,0] x+1/2,0,1/2 [u,0,0] 0,1/2,x+1/2 [0,0,u] 0,1/2,x+1/2 [0,0,u]

12 g 2.. x,1/2,0 [u,0,0] x,1/2,0 [u,0,0] 0,x,1/2 [0,u,0] 0,x,1/2 [0,u,0]

1/2,0,x [0,u,0] 1/2,0,x [0,u,0] 0,x+1/2,1/2 [0,u,0] 0,x+1/2,1/2 [0,u,0]

x+1/2,1/2,0 [u,0,0] x+1/2,1/2,0 [u,0,0] 1/2,0,x+1/2 [0,u,0] 1/2,0,x+1/2 [0,u,0]

12 f 2.. x,0,0 [u,0,0] x,0,0 [u,0,0] 0,x,0 [0,u,0] 0,x,0 [0,u,0]

0,0,x [0,0,u] 0,0,x [0,0,u] 1/2,x+1/2,1/2 [0,u,0] 1/2,x+1/2,1/2 [0,u,0]

x+1/2,1/2,1/2 [u,0,0] x+1/2,1/2,1/2 [u,0,0] 1/2,1/2,x+1/2 [0,u,0] 1/2,1/2,x+1/2 [0,u,0]
8  e  3.  x,x,x [u,u,u]  
  x,x,x [u,u,u]  
  x+1/2,x+1/2,x+1/2 [u,u,u]  
  x+1/2,x+1/2,x+1/2 [u,u,u]

6  d  4  1/4,0,1/2 [u,0,0]  
  1/2,3/4,0 [0,u,0]  
  0,1/2,1/4 [0,0,u]  
  1/2,3/4,0 [0,u,0]  
  0,1/2,1/4 [0,0,u]  
  1/2,3/4,0 [0,u,0]  
  0,1/2,1/4 [0,0,u]  
  1/2,0,1/4 [0,0,u]  
  1/2,0,3/4 [0,0,u]

6  c  4  1/4,1/2,0 [u,0,0]  
  0,3/4,1/2 [0,u,0]  
  0,1/2,0 [0,0,0]  
  1/2,0,0 [0,0,0]  
  0,1/2,0 [0,0,0]  
  1/2,0,0 [0,0,0]  
  0,1/2,0 [0,0,0]  
  1/2,0,0 [0,0,0]

2  a  23.  0,0,0 [0,0,0]  
  1/2,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4'm'm
a* = a  b* = b
Origin at 1/2,0,z

Along [1,1,1]  p31m
a* = (2a - b - c)/3  b* = (-a + 2b - c)/3
Origin at x,x,x

Along [1,1,0]  p21m
a* = (-a + b)/2  b* = c/2
Origin at x,x,0
Origin at 231°

Asymmetric unit

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad z \leq \min(x,y)\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 0,1/2,0 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \\
(1,0,0,0) & \quad (2) & \quad 2,0,0 \, z \\
(2,0,0,0) & \quad (3) & \quad 2,0,0 \, y,0 \\
(2,0,0,0) & \quad (4) & \quad 2,0,0 \, x,0,0 \\
(2,0,0,0) & \quad (5) & \quad 3^+ \, x,x,x \\
(3,xyz,0,0,0) & \quad (6) & \quad 3^+ \, x,x,x \\
(3,xyz,0,0,0) & \quad (7) & \quad 3^+ \, x,x,x \\
(3,xyz,0,0,0) & \quad (8) & \quad 3^- \, x,x,x \\
(3,xyz,0,0,0) & \quad (9) & \quad 3^- \, x,x,x \\
(3,xyz^{-1},0,0,0) & \quad (10) & \quad 3^- \, x,x,x \\
(3,xyz,0,0,0) & \quad (11) & \quad 3^- \, x,x,x \\
(3,xyz,0,0,0) & \quad (12) & \quad 3^- \, x,x,x
\end{align*}
\]
Continued

continued 218.2.1586 & P43n1'

(13) n (1/2,1/2,1/2) x,x,z
(m_{xy} | 1/2,1/2,1/2)

(14) c (0,0,1/2) x+1/2,x,z
(m_{xy} | 1/2,1/2,1/2)

(15) 4^+ 1/2,0,z;1/2,0,1/4
(4 | 1/2,1/2,1/2)

(16) 4^- 0,1/2,z; 0,1/2,1/4
(4^- | 1/2,1/2,1/2)

(17) n (1/2,1/2,1/2) x,y,y
(m_{yz} | 1/2,1/2,1/2)

(18) 4^- x,1/2,0; 1/4,1/2,0
(4^- | 1/2,1/2,1/2)

(19) 4^- x,0,1/2; 1/4,0,1/2
(4^- | 1/2,1/2,1/2)

(20) a (1/2,0,0) x,y+1/2,y
(m_{yz} | 1/2,1/2,1/2)

(21) n (1/2,1/2,1/2) x,y,x
(m_{xz} | 1/2,1/2,1/2)

(22) 4^- 1/2,y,0; 1/2,1/4,0
(4^- | 1/2,1/2,1/2)

(23) b (0,1/2,0) x+1/2,y,x
(m_{xz} | 1/2,1/2,1/2)

(24) 4^- 0,y,1/2; 0,1/4,1/2
(4^- | 1/2,1/2,1/2)

For 1' + set

(1) 1'
(1' | 0,0,0')

(3) 2' 0,y,0
(2 | 0,0,0')

(5) 3' x,x,x
(3 | 0,0,0')

(6) 3' x,x,x
(3 | 0,0,0')

(7) 3' x,x,x
(3 | 0,0,0')

(9) 3' x,x,x
(3 | 0,0,0')

(10) 3' x,x,x
(3 | 0,0,0')

(11) 3' x,x,x
(3 | 0,0,0')

(12) 3' x,x,x
(3 | 0,0,0')

(13) n' (1/2,1/2,1/2) x,x,z
(m_{xy} | 1/2,1/2,1/2')

(14) c' (0,0,1/2) x+1/2,x,z
(m_{xy} | 1/2,1/2,1/2')

(15) 4' 1/2,0,z;1/2,0,1/4
(4 | 1/2,1/2,1/2')

(16) 4' 0,1/2,z; 0,1/2,1/4
(4^- | 1/2,1/2,1/2')

(17) n' (1/2,1/2,1/2) x,y,y
(m_{yz} | 1/2,1/2,1/2')

(18) 4' x,1/2,0; 1/4,1/2,0
(4^- | 1/2,1/2,1/2')

(19) 4' x,0,1/2; 1/4,0,1/2
(4^- | 1/2,1/2,1/2')

(20) a (1/2,0,0) x,y+1/2,y
(m_{yz} | 1/2,1/2,1/2')

(21) n' (1/2,1/2,1/2) x,y,x
(m_{xz} | 1/2,1/2,1/2')

(22) 4' 1/2,y,0; 1/2,1/4,0
(4^- | 1/2,1/2,1/2')

(23) b' (0,1/2,0) x+1/2,y,x
(m_{xz} | 1/2,1/2,1/2')

(24) 4' 0,y,1/2; 0,1/4,1/2
(4^- | 1/2,1/2,1/2')

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

24 i 11'

1 + 1' +

(1) x,y,z [0,0,0]

(2) x,y,z [0,0,0]

(3) x,y,z [0,0,0]

(4) x,y,z [0,0,0]

(5) z,x,y [0,0,0]

(6) z,x,y [0,0,0]

(7) z,x,y [0,0,0]

(8) z,x,y [0,0,0]

(9) y,z,x [0,0,0]

(10) y,z,x [0,0,0]

(11) y,z,x [0,0,0]

(12) y,z,x [0,0,0]

(13) y+1/2,x+1/2,z+1/2 [0,0,0]

(14) y+1/2,x+1/2,z+1/2 [0,0,0]

(15) y+1/2,x+1/2,z+1/2 [0,0,0]

(16) y+1/2,x+1/2,z+1/2 [0,0,0]

(17) x+1/2,z+1/2,y+1/2 [0,0,0]

(18) x+1/2,z+1/2,y+1/2 [0,0,0]

(19) x+1/2,z+1/2,y+1/2 [0,0,0]

(20) x+1/2,z+1/2,y+1/2 [0,0,0]

(21) z+1/2,y+1/2,x+1/2 [0,0,0]

(22) z+1/2,y+1/2,x+1/2 [0,0,0]

(23) z+1/2,y+1/2,x+1/2 [0,0,0]

(24) z+1/2,y+1/2,x+1/2 [0,0,0]
<p>| | | | | | |</p>
<table>
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<tbody>
<tr>
<td>12</td>
<td>h</td>
<td>2..1'</td>
<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
<td>1/2,x,0 [0,0,0]</td>
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<td>0,1/2,x [0,0,0]</td>
<td>0,1/2,x [0,0,0]</td>
<td>1/2,x+1/2,0 [0,0,0]</td>
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<td>x+1/2,0,1/2 [0,0,0]</td>
<td>x+1/2,0,1/2 [0,0,0]</td>
<td>0,1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>12</td>
<td>g</td>
<td>2..1'</td>
<td>x,1/2,0 [0,0,0]</td>
<td>x,1/2,0 [0,0,0]</td>
<td>0,x,1/2 [0,0,0]</td>
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<td>1/2,0,x [0,0,0]</td>
<td>0,x+1/2,1/2 [0,0,0]</td>
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<td>x+1/2,1/2,2 [0,0,0]</td>
<td>1/2,0,x+1/2 [0,0,0]</td>
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<tr>
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<td>f</td>
<td>2..1'</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
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<td>0,0,x [0,0,0]</td>
<td>1/2,x+1/2,1/2 [0,0,0]</td>
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<td>x+1/2,1/2,2 [0,0,0]</td>
<td>1/2,1/2,x+1/2 [0,0,0]</td>
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<td>4</td>
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<td>.3.1'</td>
<td>x,x,x [0,0,0]</td>
<td>x,x,x [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
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<td>x,x,x [0,0,0]</td>
<td>x,x,x [0,0,0]</td>
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<tr>
<td>6</td>
<td>d</td>
<td>4 1'</td>
<td>1/4,0,1/2 [0,0,0]</td>
<td>3/4,0,1/2 [0,0,0]</td>
<td>1/2,1/4,0 [0,0,0]</td>
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<td>1/2,3/4,0 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
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<tr>
<td>6</td>
<td>c</td>
<td>4 1'</td>
<td>1/4,1/2,0 [0,0,0]</td>
<td>3/4,1/2,0 [0,0,0]</td>
<td>01/4,1/2 [0,0,0]</td>
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<td>0,3/4,1/2 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
<td>1/2,0,3/4 [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td>222..1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,1,2/0 [0,0,0]</td>
</tr>
<tr>
<td></td>
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<td>0,1/2,0 [0,0,0]</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>23.1'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1] p4mm1':**  
  \[a^* = a \quad b^* = b\]
  Origin at 1/2,0,z

- **Along [1,1,1] p31m1':**  
  \[a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3\]
  Origin at x,x,x

- **Along [1,1,0] p1m11':**  
  \[a^* = (-a + b)/2 \quad b^* = c/2\]
  Origin at x,x,0
Origin at 23

Asymmetric unit

\[0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad z \leq \min(x, y)\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 0,1/2,0 & \quad 1/2,1/2,1/2 \\
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) \quad & 1 \\
(1) \quad & 0,0,0 \\
\left(1 \right| 0,0,0) \\
(2) \quad & 0,0,z \\
\left(2 \right| 0,0,0) \\
(2_y) \quad & 0,y,0 \\
\left(2_y \right| 0,0,0) \\
(3) \quad & x,0,0 \\
\left(3_x \right| 0,0,0) \\
(4) \quad & 0,0,z \\
\left(2_z \right| 0,0,0) \\
(5) \quad & x,x,x \\
\left(3_{xyz} \right| 0,0,0) \\
(6) \quad & x,x,x \\
\left(3_{xyz}^{-1} \right| 0,0,0) \\
(7) \quad & x,x,x \\
\left(3_{xyz}^{-1} \right| 0,0,0) \\
(8) \quad & x,x,x \\
\left(3_{xyz}^{-1} \right| 0,0,0) \\
(9) \quad & x,x,x \\
\left(3_{xyz}^{-1} \right| 0,0,0) \\
(10) \quad & x,x,x \\
\left(3_{xyz}^{-1} \right| 0,0,0) \\
(11) \quad & x,x,x \\
\left(3_{xyz}^{-1} \right| 0,0,0) \\
(12) \quad & x,x,x \\
\left(3_{xyz}^{-1} \right| 0,0,0) \\
\end{align*}
\]
Continued

(13) n' (1/2,1/2,1/2) x,x,z
(14) c' (0,0,1/2) x+1/2,x,x,z
(15) 4' ' 1/2,0,z;1/2,0,1/4
(16) 4' ' 0,1/2,z; 0,1/2,1/4
(4' z' |1/2,1/2,1/2')

(17) n' (1/2,1/2,1/2) x,y,y
(18) 4' ' x,1/2,0; 1/4,1/2,0
(19) 4' ' x,0,1/2; 1/4,0,1/2
(4' x' |1/2,1/2,1/2')

(21) n' (1/2,1/2,1/2) x,y,x
(22) 4' ' 1/2, y,0; 1/2,1/4,0
(23) b' (0,1/2,0) x+1/2,x,x
(24) 4' ' 0,y,1/2; 0,1/4,1/2
(4' y |1/2,1/2,1/2')

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13).

Positions

Continuity
Wyckoff letter,
Site Symmetry.

24 i 1

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) x,y,z [u,v,w]
(4) x,y,z [u,v,w]

(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]

(9) y,z,x [v,w,u]
(10) y,z,x [v,w,u]
(11) y,z,x [v,w,u]
(12) y,z,x [v,w,u]

(13) y+1/2,x+1/2,z+1/2 [v,w,u]
(14) y+1/2,x+1/2,z+1/2 [v,w,u]
(15) y+1/2,x+1/2,z+1/2 [v,w,u]
(16) y+1/2,x+1/2,z+1/2 [v,w,u]

(17) x+1/2,z+1/2,y+1/2 [u,w,v]
(18) x+1/2,z+1/2,y+1/2 [u,w,v]
(19) x+1/2,z+1/2,y+1/2 [u,w,v]
(20) x+1/2,z+1/2,y+1/2 [u,w,v]

(21) z+1/2,y+1/2,x+1/2 [w,v,u]
(22) z+1/2,y+1/2,x+1/2 [w,v,u]
(23) z+1/2,y+1/2,x+1/2 [w,v,u]
(24) z+1/2,y+1/2,x+1/2 [w,v,u]

12 h 2..
x,0,1/2 [u,0,0]
  x,0,1/2 [u,0,0]
  1/2,x,0 [0,u,0]
  1/2,x,0 [0,u,0]

  0,1/2,x [0,0,u]
  0,1/2,x [0,0,u]
  1/2,x+1/2,0 [0,u,0]
  1/2,x+1/2,0 [0,u,0]

  x+1/2,0,1/2 [u,0,0]
  x+1/2,0,1/2 [u,0,0]
  0,1/2,x+1/2 [0,u,0]
  0,1/2,x+1/2 [0,u,0]

12 g 2..
x,1/2,0 [u,0,0]
  x,1/2,0 [u,0,0]
  0,x,1/2 [0,u,0]
  0,x,1/2 [0,u,0]

  1/2,0,x [0,0,u]
  1/2,0,x [0,0,u]
  0,x+1/2,1/2 [0,u,0]
  0,x+1/2,1/2 [0,u,0]

  x+1/2,1/2,0 [u,0,0]
  x+1/2,1/2,0 [u,0,0]
  1/2,0,x+1/2 [0,u,0]
  1/2,0,x+1/2 [0,u,0]

12 f 2..
x,0,0 [u,0,0]
  x,0,0 [u,0,0]
  0,x,0 [0,u,0]
  0,x,0 [0,u,0]

  0,0,x [0,0,u]
  0,0,x [0,0,u]
  1/2,x+1/2,1/2 [0,u,0]
  1/2,x+1/2,1/2 [0,u,0]

  x+1/2,1/2,1/2 [u,0,0]
  x+1/2,1/2,1/2 [u,0,0]
  1/2,1/2,x+1/2 [0,u,0]
  1/2,1/2,x+1/2 [0,u,0]

4 e .3.
x,x,x [u,u,u]
  x,x,x [u,u,u]
  x,x,x [u,u,u]

  x,x,x [u,u,u]
  x,x,x [u,u,u]
  x+1/2,x+1/2,x+1/2 [u,u,u]
  x+1/2,x+1/2,x+1/2 [u,u,u]

  x+1/2,x+1/2,x+1/2 [u,u,u]
  x+1/2,x+1/2,x+1/2 [u,u,u]
Symmetry of Special Projections

Along [0,0,1] p4m' m'

\[ a^* = a \quad b^* = b \]

Origin at 1/2,0,z

Along [1,1,1] p31m'

\[ a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \]

Origin at x,x,x

Along [1,1,0] p1m'1

\[ a^* = (-a + b)/2 \quad b^* = c/2 \]

Origin at x,x,0
Origin at 23

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad -y \leq z \leq y \]

Vertices

\begin{align*}
0,0,0 & \quad 1/2,0,0 \\
1/4,1/4,1/4 & \quad 1/4,1/4,-1/4
\end{align*}

Symmetry Operations

For \((0,0,0) + \text{set} \)

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 2 \quad 0,y,0 \\
(4) & \quad 2 \quad x,0,0 \\
(5) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^1 | 0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1} | 0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz} | 0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1} | 0,0,0) \\
(9) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz} | 0,0,0) \\
(10) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz}^{-1} | 0,0,0) \\
(11) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz} | 0,0,0) \\
(12) & \quad 3^- \quad x,x,x \\
& \quad (3_{xyz}^{-1} | 0,0,0)
\end{align*}
<table>
<thead>
<tr>
<th>Formula</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n(1/2,1/2,1/2) \ x,x,z$</td>
<td>$m_{xy}</td>
</tr>
<tr>
<td>$c(0,0,1/2) \ x+1/2,x,z$</td>
<td>$m_{xy}</td>
</tr>
<tr>
<td>$4^+ \ 1/2,0,z;1/2,0,1/4$</td>
<td>$4_z</td>
</tr>
<tr>
<td>$4^- \ 0,1/2,z;0,1/2,1/4$</td>
<td>$4_z^{-1}</td>
</tr>
<tr>
<td>$a(1/2,0,0) \ x,y+1/2,y$</td>
<td>$m_{yz}</td>
</tr>
<tr>
<td>$b(0,1/2,0) \ x,y,x$</td>
<td>$m_{xz}</td>
</tr>
</tbody>
</table>

For $(0,1/2,1/2) +$ set

<table>
<thead>
<tr>
<th>Formula</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t(0,1/2,1/2)$</td>
<td>$0,1/2,1/2$</td>
</tr>
<tr>
<td>$2(0,0,1/2) \ 0,1/4,z$</td>
<td>$2_z</td>
</tr>
<tr>
<td>$2(0,1/2,0) \ 0,y,1/4$</td>
<td>$2_y</td>
</tr>
<tr>
<td>$2(1/2,0,0) \ x,y,y$</td>
<td>$2_{xyz}</td>
</tr>
<tr>
<td>$g(1/4,0,1/4) \ x+1/4,x,z$</td>
<td>$m_{yz}</td>
</tr>
<tr>
<td>$g(1/4,0,-1/4) \ x+1/4,x,z$</td>
<td>$m_{yz}</td>
</tr>
<tr>
<td>$a(1/2,0,0) \ x,y,y$</td>
<td>$m_{yz}</td>
</tr>
<tr>
<td>$g(1/4,0,1/4) \ x+1/4,y,x$</td>
<td>$m_{xz}</td>
</tr>
</tbody>
</table>

For $(1/2,0,1/2) +$ set

<table>
<thead>
<tr>
<th>Formula</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t(1/2,0,1/2)$</td>
<td>$1/2,0,1/2$</td>
</tr>
<tr>
<td>$2(0,0,1/2) \ 1/4,0,z$</td>
<td>$2_z</td>
</tr>
<tr>
<td>$2(0,1/2,0) \ 1/4,y,1/4$</td>
<td>$2_y</td>
</tr>
<tr>
<td>$2(1/2,0,0) \ x,0,1/4$</td>
<td>$2_{xyz}</td>
</tr>
<tr>
<td>$g(-1/4,1/4,0) \ x+1/4,x,z$</td>
<td>$m_{xy}</td>
</tr>
<tr>
<td>$g(1/4,1/4,0) \ x+1/4,x,z$</td>
<td>$m_{xy}</td>
</tr>
<tr>
<td>$g(0,1/4,1/4) \ x,y+1/4,y$</td>
<td>$m_{yz}</td>
</tr>
<tr>
<td>$g(0,1/4,-1/4) \ x+1/4,y,x$</td>
<td>$m_{yz}</td>
</tr>
<tr>
<td>$b(0,1/2,0) \ x,y,z$</td>
<td>$m_{xz}</td>
</tr>
</tbody>
</table>

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Continued

\[\begin{align*}
(1) & \quad t(1/2,1/2,0) \\
(5) & \quad 3^* (1/3,1/3,1/3) \quad x+1/6, x+1/3, x \\
& \quad (3_{xyz}) [1/2,1/2,0] \\
(9) & \quad 3^* (1/3,1/3,1/3) \quad x+1/6, x+1/3, x \\
& \quad (3_{xyz}) [-1/2,1/2,0] \\
(13) & \quad c(0,0,1/2) \quad x,x,z \\
& \quad (m_{xz}) [0,0,1/2] \\
(17) & \quad g(0,1/4,1/4) \quad x,-1/4,1/4; 0,-1/4,1/4 \\
& \quad (m_{yz}) [0,0,1/2] \\
(21) & \quad g(1/4,0,1/4) \quad x+1/4, y+1/4, 0 \\
& \quad (m_{xz}) [0,0,1/2] \\
\end{align*}\]

Generators selected 
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,0,1/2); t(1/2,0,1/2); (2); (3); (5); (13).

### Positions

\[
\begin{align*}
\text{Multiplicity,} & \quad \text{Wyckoff letter,} \\
\text{Site Symmetry.} & \quad \text{Coordinates} \\
\end{align*}
\]

\[
\begin{align*}
\text{96} & \quad h \quad 1 \\
(1) & \quad x,y,z \quad [u,v,w] \\
(5) & \quad z,x,y \quad [w,u,v] \\
(9) & \quad y,z,x \quad [v,w,u] \\
(13) & \quad y+1/2, x+1/2, z+1/2 \quad [v,u,w] \\
(17) & \quad x+1/2, z+1/2, y+1/2 \quad [u,w,v] \\
(21) & \quad z+1/2, y+1/2, x+1/2 \quad [w,v,u] \\
\end{align*}
\]

\[
\begin{align*}
48 & \quad g \quad 2.. \\
& \quad x,1/4,1/4 [u,0,0] \\
& \quad 1/4,1/4 [u,0,0] \\
& \quad 1/4,1/4, x [0,0,u] \\
& \quad x+1/2,3/4,3/4 [u,0,0] \\
\end{align*}
\]

\[
\begin{align*}
48 & \quad f \quad 2.. \\
& \quad x,0,0 [u,0,0] \\
& \quad x,0,0 [0,u,0] \\
& \quad 0,x,0 [u,0,0] \\
& \quad 0,x,0 [0,u,0] \\
\end{align*}
\]

\[
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\]
Continued

32 e .3. \(x,x,x [u,u,u]\) \(\overline{x},x,x [u,u,u]\) 
\(\overline{x},x,x [u,u,u]\) \(x,x,x [u,u,u]\)
\(x+1/2,x+1/2,x+1/2 [u,u,u]\) 
\(\overline{x}+1/2,\overline{x}+1/2,\overline{x}+1/2 [u,u,u]\) 
\(\overline{x}+1/2,\overline{x}+1/2,\overline{x}+1/2 [u,u,u]\)

24 d \(\overline{4}\) \(1/4,0,0 [u,0,0]\) \(3/4,0,0 [\overline{u},0,0]\) \(0,1/4,0 [0,u,0]\)
\(0,3/4,0 [0,\overline{u},0]\) \(0,0,1/4 [0,0,u]\) \(0,0,3/4 [0,0,\overline{u}]\)

24 c \(\overline{4}\) \(0,1/4,1/4 [u,0,0]\) \(0,3/4,1/4 [\overline{u},0,0]\) \(1/4,0,1/4 [0,u,0]\)
\(1/4,0,3/4 [0,\overline{u},0]\) \(1/4,1/4 [0,0,u]\) \(3/4,1/4 [0,0,\overline{u}]\)

8 b 23. \(1/4,1/4,1/4 [0,0,0]\) \(3/4,3/4,3/4 [0,0,0]\)

8 a 23. \(0,0,0 [0,0,0]\) \(1/2,1/2,1/2 [0,0,0]\)

**Symmetry of Special Projections**

Along \([0,0,1]\) \(p4'm'm\)
\(a^* = a/2\) \(b^* = b/2\)
Origin at 0,0,z

Along \([1,1,1]\) \(p31m\)
\(a^* = (2a - b - c)/6\) \(b^* = (-a + 2b - c)/6\)
Origin at x,x,x

Along \([1,1,0]\) \(p_2'1m1\)
\(a^* = (-a + b)/2\) \(b^* = c/2\)
Origin at x-1/4,x+1/4,0
Origin at 231°

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad -1/4 \leq z \leq 1/4; \quad y \leq \min(x, 1/2-x); \quad -y \leq z \leq y\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\begin{align*}
(1) & \quad 1 \\
(2) & \quad (2) \quad 0,0,z \quad (2) \quad 0,y,0 \quad (4) \quad 2 \quad x,0,0 \\
(5) & \quad 3^+ \quad x,x,x \quad (3_{xyz}^+ | 0,0,0) \quad (7) \quad 3^+ \quad x,x,x \quad (3_{xyz}^{-1} | 0,0,0) \quad (8) \quad 3^+ \quad x,x,x \quad (3_{xyz}^{-1} | 0,0,0) \\
(9) & \quad 3^- \quad x,x,x \quad (3_{xyz}^{-1} | 0,0,0) \quad (10) \quad 3^- \quad x,x,x \quad (3_{xyz}^{-1} | 0,0,0) \quad (11) \quad 3^- \quad x,x,x \quad (3_{xyz}^{-1} | 0,0,0) \quad (12) \quad 3^- \quad x,x,x \quad (3_{xyz}^{-1} | 0,0,0)
\end{align*}
Continued

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1 1/2,1/2,0)
(2) 2' 1/4,1/4,z
(2' 1/2,1/2,0)
(3) 2' (0,1/2,0) 1/4,y,0
(3' 1/2,1/2,0)
(4) 2' (1/2,0,0) x,1/4,0
(2' 1/2,1/2,0)

(5) 3' (1/3,1/3,1/3)
(3xyz 1/2,1/2,0)
(6) 3' x+1/2,x,x
(3xyz 1/2,1/2,0)
(7) 3' x+1/2,x,x
(3xyz 1/2,1/2,0)
(8) 3' (1/3,1/3,-1/3)
(3xyz 1/2,1/2,0)

For (0,0,0)' + set

(1) 1'
(1 0,0,0)' 0,0,z
(2) 2' 0,0,z
(2 0,0,0)' 0,0,0)
(3) 2' 0,y,0
(3' 0,0,0)'
(4) 2' 0,0,0)
(2' 0,0,0)'

(5) 3' x,x,x
(3xyz 0,0,0)'
(6) 3' x,x,x
(3xyz 0,0,0)'
(7) 3' x,x,x
(3xyz 0,0,0)'
(8) 3' x,x,x
(3xyz 0,0,0)'

(9) 3' x,x,x
(3xyz 0,0,0)'
(10) 3' x,x,x
(3xyz 0,0,0)'
(11) 3' x,x,x
(3xyz 0,0,0)'
(12) 3' x,x,x
(3xyz 0,0,0)'

(13) n' (1/2,1/2,1/2)
(x,x,z
(mxyz 1/2,1/2,1/2)'
(14) c' (0,0,1/2) x+1/2,x,z
(mxyz 1/2,1/2,1/2)'
(15) 4' x+1/2,0,0; x+1/2,1/2,0,1/4
(4' 1/2,1/2,1/2)'
(16) 4' x+1/2,0,0; x+1/2,1/2,1/4
(4' 1/2,1/2,1/2)'

(17) n' (1/2,1/2,1/2)
(x,y,y
(mxyz 1/2,1/2,1/2)'
(18) 4' x+1/2,0,1/4,1/4,0,1/2
(4' 1/2,1/2,1/2)'
(19) 4' x+1/2,0,1/4,1/4,0,1/2
(4' 1/2,1/2,1/2)'
(20) a' (1/2,0,0) x,y+1/2,y
(mxyz 1/2,1/2,1/2)'

(21) n' (1/2,1/2,1/2)
(x,y,x
(mxyz 1/2,1/2,1/2)'
(22) 4' x+1/2,0,y; 1/2,1/4,0
(4' 1/2,1/2,1/2)'
(23) b' (0,1/2,0) x+1/2,y,x
(mxyz 1/2,1/2,1/2)'
(24) 4' x+1/2,0,y; 1/2,1/4,0
(4' 1/2,1/2,1/2)'

(1) t' (0,1/2,1/2)
(1 0,1/2,1/2)'
(2) 2' (0,0,1/2) 0,1/4,z
(2' 0,1/2,1/2)'
(3) 2' (0,1/2,0) 0,y,1/4
(3' 0,1/2,1/2)'
(4) 2' x,1/4,1/4
(2' 0,1/2,1/2)'

(5) 3' (1/3,1/3,1/3)
(x+1/3,x+1/6,x
(3xyz 0,1/2,1/2)'
(6) 3' x+1/2,x,x
(3xyz 0,1/2,1/2)'
(7) 3' x+1/2,x,x
(3xyz 0,1/2,1/2)'
(8) 3' x+1/2,x,x
(3xyz 0,1/2,1/2)'

(9) 3' (1/3,1/3,1/3)
(x+1/6,x+1/6,x
(3xyz 0,1/2,1/2)'
(10) 3' x+1/2,x,x
(3xyz 0,1/2,1/2)'
(11) 3' x+1/2,x,x
(3xyz 0,1/2,1/2)'
(12) 3' x+1/2,x,x
(3xyz 0,1/2,1/2)'

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Continued

For $\langle 1/2,0,1/2 \rangle + \text{set}$

(1) $t'$ (1/2,1/2,0)  
(1/2,1/2,0)' 

(2) $2'$ (0,0,1/2)  1/4,0,z 
(2' \mid 1/2,0,1/2)' 

(3) $2'$ 1/4,y,1/4 
(2' \mid 1/2,0,1/2)' 

(4) $2'$ (1/2,0,0)  x,0,1/4 
(2' \mid 1/2,0,1/2)' 

(5) $3'$ (1/3,1,3/3)  

x+1/6,x-1/6,x  
(3' \mid x+1/6,x+1/6,x)' 

(6) $3'$ (1/3,-1/3,1/3)  

x+1/6,x-1/6,x  
(3' \mid x+1/6,x+1/6,x)' 

(7) $3'$ x+1/2,x-1/2,x 
(3' \mid x+1/2,x+1/2,x)' 

(8) $3'$ x+1/2,x+1/2,x 
(3' \mid x+1/2,x+1/2,x)' 

(9) $3'$ (1/3,3,1/3)  

x+1/6,x-1/6,x  
(3' \mid x+1/6,x+1/6,x)' 

(10) $3'$ x+1/2,x-1/2,x  
(3' \mid x+1/2,x+1/2,x)' 

(11) $3'$ x+1/2,x-1/2,x 
(3' \mid x+1/2,x+1/2,x)' 

(12) $3'$ (1/3,-1,3/3)  

x+1/6,x+1/3,x  
(3' \mid x+1/6,x+1/3,x)' 

(13) $g'$ (1/4,1/4,0)  x-1/4,x,z 
(m'_{xz} \mid 0,1/2,0)' 

(14) $g'$ (1/4,-1/4,0)  x+1/4,x,z 
(m'_{xy} \mid 0,1/2,0)' 

(15) $4^{++}$ 1/4,1/4,z; 1/4,1/4,0 
(4' \mid z,1/2,0,0)' 

(16) $4^{++}$ 1/4,1/4,z; 1/4,1/4,0 
(4' \mid z,1/2,0,0)' 

(17) $g'$ (0,1/4,1/4)  x,y,y 
(m'_{yz} \mid 0,1/2,0)' 

(18) $g'$ (0,1/4,-1/4)  x,y,y 
(m'_{yz} \mid 0,1/2,0)' 

(19) $4^{++}$ 1/4,1/4,y; 1/4,0,1/4 
(4' \mid y,0,1/2,0)' 

(20) $g'$ (0,1/4,-1/4)  x,y,y 
(m'_{yz} \mid 0,1/2,0)' 

(21) $b'$ (0,1/2,0)  x,y,x 
(m'_{xz} \mid 0,1/2,0)' 

(22) $b'$ (0,1/2,0)  x,y,x 
(m'_{xz} \mid 0,1/2,0)' 

(23) $b'$ (0,1/2,0)  x,y,x 
(m'_{xz} \mid 0,1/2,0)' 

(24) $4^{++}$ 0,y,0; 0,1/4,0 
(4' \mid y,0,1/2,0)' 

For $\langle 1/2,1/2,0 \rangle + \text{set}$

(1) $t'$ (1/2,1/2,0)  
(1/2,1/2,0)' 

(2) $2'$ 1/4,1/4,z 
(2' \mid 1/2,1/2,0)' 

(3) $2'$ (0,1/2,0)  1/4,y,0 
(2' \mid 1/2,1/2,0)' 

(4) $2'$ (1/2,0,0)  x,1/4,0 
(2' \mid 1/2,1/2,0)' 

(5) $3'$ (1/3,1/3,1/3)  

x+1/6,x+1/3,x  
(3' \mid x+1/6,x+1/3,x)' 

(6) $3'$ x+1/2,x-1/2,x  
(3' \mid x+1/2,x+1/2,x)' 

(7) $3'$ x+1/2,x-1/2,x  
(3' \mid x+1/2,x+1/2,x)' 

(8) $3'$ (1/3,1/3,1/3)  

x+1/6,x+1/3,x  
(3' \mid x+1/6,x+1/3,x)' 

(9) $3'$ (1/3,1/3,1/3)  

x+1/6,x+1/3,x  
(3' \mid x+1/6,x+1/3,x)' 

(10) $3'$ x+1/2,x-1/2,x  
(3' \mid x+1/2,x+1/2,x)' 

(11) $3'$ x+1/2,x-1/2,x  
(3' \mid x+1/2,x+1/2,x)' 

(12) $3'$ (1/3,1/3,1/3)  

x+1/6,x+1/3,x  
(3' \mid x+1/6,x+1/3,x)' 

(13) $c'$ (0,0,1/2)  x,x,z 
(m'_{xy} \mid 0,1/2,0)' 

(14) $c'$ (0,0,1/2)  x,x,z 
(m'_{xy} \mid 0,1/2,0)' 

(15) $4^{++}$ 0,z; 0,0,1/4 
(4' \mid 0,0,1/2)' 

(16) $4^{++}$ 0,z; 0,0,1/4 
(4' \mid 0,0,1/2)' 

(17) $g'$ (0,1/4,1/4)  x,y,-1/4,y 
(m'_{yz} \mid 0,1/2,0)' 

(18) $g'$ (0,1/4,-1/4)  x,y,-1/4,y 
(m'_{yz} \mid 0,1/2,0)' 

(19) $4^{++}$ x,-1/4,1/4; 0,-1/4,1/4 
(4' \mid 0,1/2,0)' 

(20) $g'$ (0,-1/4,1/4)  x,y+1/4,y 
(m'_{yz} \mid 0,1/2,0)' 

(21) $g'$ (1/4,0,1/4)  x-1/4,y,x 
(m'_{xz} \mid 0,0,1/2)' 

(22) $g'$ (1/4,0,1/4)  x-1/4,y,x 
(m'_{xz} \mid 0,0,1/2)' 

(23) $g'$ (1/4,0,1/4)  x+1/4,y,x 
(m'_{xz} \mid 0,0,1/2)' 

(24) $4^{++}$ -1/4,1/4,y; -1/4,0,1/4 
(4' \mid y,0,1/2,0)' 

Generators selected  
(1); (1,0,0); (0,0,1); (t,0,1,0); (t,0,1/2,1/2); (t,1/2,0,1/2); (2); (3); (5); (13); 1'.
### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) + (0,0,0)' + (0,1/2,1/2)' + (1/2,0,1/2)' + (1/2,1/2,0)'</td>
<td>(1) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>96 h 11'</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(3) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(5) z,x,y [0,0,0]</td>
<td>(7) z,x,y [0,0,0]</td>
</tr>
<tr>
<td>(9) y,z,x [0,0,0]</td>
<td>(11) y,z,x [0,0,0]</td>
</tr>
<tr>
<td>(13) y+1/2,x+1/2,z+1/2 [0,0,0] (14) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
<td>(15) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(17) x+1/2,z+1/2,y+1/2 [0,0,0] (18) x+1/2,z+1/2,y+1/2 [0,0,0]</td>
<td>(19) x+1/2,z+1/2,y+1/2 [0,0,0]</td>
</tr>
<tr>
<td>(21) z+1/2,y+1/2,x+1/2 [0,0,0] (22) z+1/2,y+1/2,x+1/2 [0,0,0]</td>
<td>(23) z+1/2,y+1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>48 g 2..1' x,1/4,1/4 [0,0,0] x,3/4,1/4 [0,0,0] 1/4,x,1/4 [0,0,0] 1/4,x,3/4 [0,0,0]</td>
<td>(10) y,z,x [0,0,0]</td>
</tr>
<tr>
<td>1/4,1/4,x [0,0,0] 3/4,1/4,x [0,0,0] 3/4,x+1/2,3/4 [0,0,0] 1/4,x+1/2,3/4 [0,0,0]</td>
<td>(11) y,z,x [0,0,0]</td>
</tr>
<tr>
<td>x+1/2,3/4,3/4 [0,0,0] x+1/2,3/4,1/4 [0,0,0] 3/4,3/4,x+1/2 [0,0,0] 3/4,1/4,x+1/2 [0,0,0]</td>
<td>(12) y,z,x [0,0,0]</td>
</tr>
<tr>
<td>48 f 2..1' x,0,0 [0,0,0] x,0,0 [0,0,0] 0,x,0 [0,0,0] 0,x,0 [0,0,0]</td>
<td>(13) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>0,0,x [0,0,0] 0,0,x [0,0,0] 1/2,x+1/2,1/2 [0,0,0] 1/2,x+1/2,1/2 [0,0,0]</td>
<td>(16) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>x+1/2,1/2,1/2 [0,0,0] x+1/2,1/2,1/2 [0,0,0] 1/2,1/2,x+1/2 [0,0,0] 1/2,1/2,x+1/2 [0,0,0]</td>
<td>(19) x+1/2,z+1/2,y+1/2 [0,0,0]</td>
</tr>
<tr>
<td>32 e .3.1' x,x,x [0,0,0] x,x,x [0,0,0] x,x,x [0,0,0] x,x,x [0,0,0]</td>
<td>(20) x+1/2,z+1/2,y+1/2 [0,0,0]</td>
</tr>
<tr>
<td>x+1/2,x+1/2,x+1/2 [0,0,0] x+1/2,x+1/2,x+1/2 [0,0,0] x+1/2,x+1/2,x+1/2 [0,0,0]</td>
<td>(24) z+1/2,y+1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>24 d 4 1' 1/4,0,0 [0,0,0] 3/4,0,0 [0,0,0] 0,1/4,0 [0,0,0] 0,1/4,0 [0,0,0]</td>
<td>(14) y+1/2,x+1/2,z+1/2 [0,0,0]</td>
</tr>
<tr>
<td>0,3/4,0 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0] 0,0,1/4 [0,0,0]</td>
<td>(17) x+1/2,z+1/2,y+1/2 [0,0,0]</td>
</tr>
<tr>
<td>24 c 4 1' 0,1/4,1/4 [0,0,0] 0,3/4,1/4 [0,0,0] 1/4,0,1/4 [0,0,0] 1/4,0,1/4 [0,0,0]</td>
<td>(18) x+1/2,z+1/2,y+1/2 [0,0,0]</td>
</tr>
<tr>
<td>1/4,0,3/4 [0,0,0] 1/4,1/4 [0,0,0] 1/4,1/4 [0,0,0] 3/4,1/4 [0,0,0]</td>
<td>(21) z+1/2,y+1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 b 23.1' 1/4,1/4,1/4 [0,0,0] 3/4,3/4,3/4 [0,0,0]</td>
<td>(22) z+1/2,y+1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 a 23.1' 0,0,0 [0,0,0] 1/2,1/2,1/2 [0,0,0]</td>
<td>(23) z+1/2,y+1/2,x+1/2 [0,0,0]</td>
</tr>
</tbody>
</table>
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Direction</th>
<th>Space Group</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0,0,1]</td>
<td>p4mm1'</td>
<td>(a^* = a/2), (b^* = b/2)</td>
</tr>
<tr>
<td>[1,1,1]</td>
<td>p31m1'</td>
<td>(a^* = (2a - b - c)/6), (b^* = (-a + 2b - c)/6)</td>
</tr>
<tr>
<td>[1,1,0]</td>
<td>p1m11'</td>
<td>(a^* = (-a + b)/2), (b^* = c/2)</td>
</tr>
</tbody>
</table>

- \(a^* = a/2\)
- \(b^* = b/2\)
- \(a^* = (2a - b - c)/6\)
- \(b^* = (-a + 2b - c)/6\)
- \(a^* = (-a + b)/2\)
- \(b^* = c/2\)
Origin at 0,0,0

Asymmetric unit

\[0 \leq x < \frac{1}{2}; \quad 0 \leq y < \frac{1}{4}; \quad -\frac{1}{4} \leq z < \frac{1}{4}; \quad y < \min(x,\frac{1}{2} - x); \quad -y < z < y\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[(1) \quad 1 \quad (2) \quad 2 \quad 0,0,z \quad (3) \quad 2 \quad 0,y,0 \quad (4) \quad 2 \quad x,0,0\]

\[(1) \quad 1 \quad (2) \quad 2 \quad 0,0,0 \quad (2) \quad 2 \quad 0,0,0 \quad (2) \quad 2 \quad 0,0,0\]

\[(5) \quad 3^+ \quad x,x,x \quad (3) \quad 3^+ \quad x,x,x \quad (4) \quad 3^- \quad x,x,x \quad (5) \quad 3^- \quad x,x,x\]

\[(6) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (3) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (4) \quad 3^- \quad \bar{x},\bar{x},\bar{x}\]

\[(7) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (3) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (4) \quad 3^- \quad \bar{x},\bar{x},\bar{x}\]

\[(8) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (3) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (4) \quad 3^- \quad \bar{x},\bar{x},\bar{x}\]

\[(9) \quad 3^- \quad x,x,x \quad (10) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (11) \quad 3^+ \quad \bar{x},\bar{x},\bar{x} \quad (12) \quad 3^- \quad \bar{x},\bar{x},\bar{x}\]

\[(3) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (3) \quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (3) \quad 3^- \quad \bar{x},\bar{x},\bar{x}\]
(13) n' (1/2,1/2,1/2) x,x,z  
(m_{xy} | 1/2,1/2,1/2)

(14) c' (0,0,1/2) x+1/2,x,z  
(m_{xy} | 1/2,1/2,1/2)

(15) 4' * 1/2,0,z; 1/2,0,1/4  
(4_{z}' | 1/2,1/2,1/2)

(16) 4' * 0,1/2,z; 0,1/2,1/4  
(4_{z}' | 1/2,1/2,1/2)

(17) n' (1/2,1/2,1/2) x,y,y  
(m_{yz} | 1/2,1/2,1/2)

(18) 4'' x,1/2,0; 1/4,1/2,0  
(4_{z}' | 1/2,1/2,1/2)

(19) 4' * x,0,1/2; 1/4,0,1/2  
(4_{z}' | 1/2,1/2,1/2)

(20) a' (1/2,0,0) x,y+1/2,y  
(m_{yz} | 1/2,1/2,1/2)

(21) n' (1/2,1/2,1/2) x,y,x  
(m_{xz} | 1/2,1/2,1/2)

(22) 4' * 1/2,y,0; 1/2,1/4,0  
(4_{y}' | 1/2,1/2,1/2)

(23) b' (0,1/2,0) x+1/2,y,x  
(m_{xz} | 1/2,1/2,1/2)

(24) 4' * 0,y,1/2; 0,1/4,1/2  
(4_{y}' | 1/2,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)  
(1 | 0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z  
(2_{z} | 0,1/2,1/2)

(3) 2 (0,1/2,0) 0,y,1/4  
(2_{y} | 0,1/2,1/2)

(4) 2 x,1/4,1/4  
(2_{x} | 0,1/2,1/2)

(5) 3* (1/3,1/3,1/3) x-1/3,x-1/6,x  
(3_{xyz} | 0,1/2,1/2)

(6) 3* x,x+1/2,x  
(3_{xyz}^{-1} | 0,1/2,1/2)

(7) 3* (-1/3,1/3,1/3) x+1/3,x-1/6,x  
(3_{xyz}^{-1} | 0,1/2,1/2)

(8) 3* x,x+1/2,x  
(3_{xyz}^{-1} | 0,1/2,1/2)

(9) 3* (1/3,1/3,1/3) x+1/6,x+1/6,x  
(3_{xyz}^{-1} | 0,1/2,1/2)

(10) 3* x+1/2,x+1/2,x  
(3_{xyz}^{-1} | 0,1/2,1/2)

(11) 3* x+1/2,x+1/2,x  
(3_{xyz}^{-1} | 0,1/2,1/2)

(12) 3* x+1/2,x+1/2,x  
(3_{xyz}^{-1} | 0,1/2,1/2)

(13) g' (1/4,1/4,0) x+1/4,x,z  
(m_{xy} | 1/2,0,0)

(14) g' (1/4,1/4,0) x+1/4,x,z  
(m_{xy} | 1/2,0,0)

(15) 4' * 1/4,1/4,z; 1/4,1/4,0  
(4_{z}' | 1/2,0,0)

(16) 4' * 1/4,1/4,z; 1/4,1/4,0  
(4_{z}' | 1/2,0,0)

(17) a' (1/2,0,0) x,y,y  
(m_{yz} | 1/2,0,0)

(18) 4' * x,0,0; 1/4,0,0  
(4_{x} | 1/2,0,0)

(19) 4' * x,0,0; 1/4,0,0  
(4_{x} | 1/2,0,0)

(20) a' (1/2,0,0) x,y,y  
(m_{yz} | 1/2,0,0)

(21) g' (1/4,0,1/4) x+1/4,y,x  
(m_{xz} | 1/2,0,0)

(22) 4' * x+1/4,y,x  
(4_{y}' | 1/2,0,0)

(23) g' (1/4,0,1/4) x+1/4,y,x  
(m_{xz} | 1/2,0,0)

(24) 4' * x+1/4,y,1/4; 1/4,0,1/4  
(4_{y}' | 1/2,0,0)

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2)  
(1 | 1/2,0,1/2)

(2) 2 (0,0,1/2) 1/4,0,z  
(2_{z} | 1/2,0,1/2)

(3) 2 (0,1/2,0) 1/4,y,1/4  
(2_{y} | 1/2,0,1/2)

(4) 2 (1/2,0,0) 0,x,1/4  
(2_{x} | 1/2,0,1/2)

(5) 3* (1/3,1/3,1/3) x+1/6,x+1/6,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(6) 3* x+1/2,x-1/2,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(7) 3* x+1/2,x-1/2,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(8) 3* x+1/2,x-1/2,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(9) 3* (1/3,1/3,1/3) x+1/6,x+1/3,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(10) 3* x+1/2,x,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(11) 3* x+1/2,x,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(12) 3* (1/3,-1/3,1/3) x-1/6,x+1/3,x  
(3_{xyz}^{-1} | 1/2,0,1/2)

(13) g' (1/4,1/4,0) x-1/4,x,z  
(m_{xy} | 1/2,0,0)

(14) g' (-1/4,1/4,0) x-1/4,x,z  
(m_{xy} | 1/2,0,0)

(15) 4' * 1/4,1/4,z; 1/4,1/4,0  
(4_{z}' | 1/2,0,0)

(16) 4' * 1/4,1/4,z; -1/4,1/4,0  
(4_{z}' | 1/2,0,0)

(17) g' (0,1/4,1/4) x,y+1/4,y  
(m_{yz} | 1/2,0,0)

(18) 4' * x,1/4,-1/4; 0,1/4,-1/4  
(4_{x} | 1/2,0,0)

(19) 4' * x,1/4,-1/4; 0,1/4,-1/4  
(4_{x} | 1/2,0,0)

(20) g' (0,1/4,-1/4) x,y+1/4,y  
(m_{yz} | 1/2,0,0)

(21) b' (0,1/2,0) x,y,x  
(m_{xz} | 1/2,0,0)

(22) 4' * x,y,0; 0,1/4,0  
(4_{y}' | 1/2,0,0)

(23) b' (0,1/2,0) x,y,x  
(m_{xz} | 1/2,0,0)

(24) 4' * 0,y,0; 0,1/4,0  
(4_{y}' | 1/2,0,0)
Continued 219.3.1590 F4'3c'
32  e  .3.  x,x,x [u,u,u]  
   x,x,x [u,u,u]  
   x,x,x [u,u,u]  
   x+1/2,x+1/2,x+1/2 [u,u,u]  
   x+1/2,x+1/2,x+1/2 [u,u,u]  
24  d  4'  1/4,0,0 [0,0,0]  
    3/4,0,0 [0,0,0]  
    0,1/4,0 [0,0,0]  
24  c  4'  0,1/4,1/4 [0,0,0]  
    0,0,1/4 [0,0,0]  
    1/4,0,3/4 [0,0,0]  
7  b  23.  1/4,1/4,1/4 [0,0,0]  
    3/4,3/4,3/4 [0,0,0]  
8  a  23.  0,0,0 [0,0,0]  
    1/2,1/2,1/2 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1]  p4m'm'  
   a* = a/2  b* = b/2  
   Origin at 0,0,z  
Along [1,1,1]  p31m'  
   a* = (2a - b - c)/6  b* = (-a + 2b - c)/6  
   Origin at x,x,x  
Along [1,1,0]  p1m'1  
   a* = (-a + b)/2  b* = c/2  
   Origin at x,x,0
**Origin** on \([1,1,1]\) at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 21 axes

**Asymmetric unit**

\[\frac{1}{4} \leq x \leq \frac{1}{2}; \quad \frac{1}{4} \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad z \leq \text{min}(x,y)\]

**Vertices**

\[
\begin{align*}
1/4, 1/4, 0 & \quad 1/2, 1/4, 0 & \quad 1/2, 1/2, 0 & \quad 1/4, 1/2, 0 \\
1/4, 1/4, 1/4 & \quad 1/2, 1/4, 1/4 & \quad 1/2, 1/2, 1/2 & \quad 1/4, 1/2, 1/4
\end{align*}
\]

**Symmetry Operations**

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\
(2) & \quad (0,0,1/2) \quad \frac{1}{4}, 0, z \\
(3) & \quad (0,1/2,0) \quad 0, y, 1/4 \\
(4) & \quad (1/2,0,0) \quad x, 1/4, 0 \\
(5) & \quad 3^+ \quad x,x,x \\
(6) & \quad 3^+ \quad \frac{x+1}{2}, x, x \\
(7) & \quad 3^+ \quad x+1/2, x-1/2, x \\
(8) & \quad 3^+ \quad x, x+1/2, x \\
(9) & \quad 3^- \quad (-1/3, 1/2, 1/3) \\
(10) & \quad 3^- \quad (1/3, 1/3, -1/3) \\
(11) & \quad (1/3, -1/3, 1/3) \\
(12) & \quad \frac{x+1}{2}, x+1/6, x \\
(13) & \quad 3xyz \quad \frac{1}{2}, 1/4, 1/4 \\
(14) & \quad (1/4, 1/4, 1/4) \quad x,x,z \\
(15) & \quad 4^+ \quad \frac{1}{2}, 1/2, 1/4; \quad 1/2, 1/4, 1/8 \\
(16) & \quad 3^- \quad 1/4, z; \quad 0, 1/4, 3/8 \\
(17) & \quad 3xyz \quad 1/4, 1/4, 1/4 \\
(18) & \quad (1/4, 1/4, 1/4) \quad x, y, y \\
(19) & \quad 4^+ \quad 1/4, 1/4, 1/4 \\
(20) & \quad (1/4, 1/4, 1/4) \quad x, y+1/2, y \\
(21) & \quad (1/4, 1/4, 1/4) \quad x, y, x \\
(22) & \quad 4^+ \quad 3/4, 3/4, 3/4 \\
(23) & \quad d \quad 3/4, 3/4, 3/4 \\
(24) & \quad 4^- \quad -1/4, y, 1/2; \quad -1/4, 3/8, 1/2 \\
\end{align*}
\]

For \((1/2,1/2,1/2) + \) set

\[
\begin{align*}
(1) & \quad t(1/2,1/2,1/2) \\
(2) & \quad 0, 1/4, z \\
(3) & \quad 1/4, y, 0 \\
(4) & \quad x, 0, 1/4 \\
(5) & \quad 3^- \quad (1/2, 1/2, 1/2) \quad x, x, x \\
(6) & \quad 3^- \quad (1/6, 1/6, 1/6) \quad x-1/6, x+1/3, x \\
(7) & \quad 3^- \quad (1/6, 1/6, 1/6) \quad x+1/6, x+1/6, x \\
(8) & \quad 3^- \quad (1/6, 1/6, 1/6) \quad x+1/3, x+1/6, x \\
(9) & \quad 3^- \quad (1/2, 1/2, 1/2) \quad x, x, x \\
(10) & \quad 3^- \quad (1/6, 1/6, 1/6) \quad x+1/6, x+1/6, x \\
(11) & \quad 3^- \quad (1/6, 1/6, 1/6) \quad x+1/3, x+1/6, x \\
(12) & \quad 3^- \quad (1/6, 1/6, 1/6) \quad x-1/6, x+1/3, x \\
(13) & \quad d \quad (3/4, 3/4, 3/4) \quad x, x, z \\
(14) & \quad d \quad (1/4, 1/4, 1/4) \quad x+1/2, x, z \\
(15) & \quad 4^+ \quad 1/2, 1/4, z; \quad 1/2, 1/4, 1/8 \\
(16) & \quad 4^- \quad 0, 1/4, z; \quad 0, 1/4, 3/8 \\
(17) & \quad d \quad (3/4, 3/4, 3/4) \quad x, y, y \\
(18) & \quad d \quad (3/4, 3/4, 3/4) \quad x+1/2, 1/4; \quad 1/8, 1/2, 1/4 \\
(19) & \quad 4^- \quad 0, 1/4, 1/8; \quad 3/8, 0, 1/4 \\
(20) & \quad d \quad (1/4, 1/4, 1/4) \quad x, y+1/2, y \\
(21) & \quad d \quad (3/4, 3/4, 3/4) \quad x, y, x \\
(22) & \quad 4^- \quad 1/4, y, 0; \quad 1/4, 0, 3/8 \\
(23) & \quad d \quad (1/4, 1/4, 1/4) \quad x, y+1/2, y; \quad 1/4, 1/8, 1/2 \\
(24) & \quad 4^- \quad 1/4, y, 1/2; \quad 1/4, 1/8, 1/2 \\
\end{align*}
\]

**Generators selected**

\(1; t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).\)
### Positions

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0) +</td>
<td>(1/2,1/2,1/2) +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x + 1/2, y + 1/2, z + 1/2 [u,v,w]</td>
</tr>
<tr>
<td>(3) x, y + 1/2, z + 1/2 [u,v,w]</td>
<td>(4) x + 1/2, y + 1/2, z [u,v,w]</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) x + 1/2, y, z + 1/2 [u,v,w]</td>
</tr>
<tr>
<td>(7) z + 1/2, x + y + 1/2 [w,u,v]</td>
<td>(8) z, x + 1/2, y + 1/2 [w,u,v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) y + 1/2, z, x + 1/2 [v,w,u]</td>
</tr>
<tr>
<td>(11) y + 1/2, z + 1/2, x [v,w,u]</td>
<td>(12) y + 1/2, z, x + 1/2 [v,w,u]</td>
</tr>
<tr>
<td>(13) y + 1/4, x + 1/4, z + 1/4 [v, w, u]</td>
<td>(14) y + 1/4, x + 3/4, z + 3/4 [v, w, u]</td>
</tr>
<tr>
<td>(15) x + 3/4, x + 1/4, z + 3/4 [u, v, w]</td>
<td>(16) y + 1/4, x + 3/4, z + 1/4 [v, u, w]</td>
</tr>
<tr>
<td>(17) x + 1/4, z + 1/4, y + 1/4 [v, w, u]</td>
<td>(18) x + 3/4, z + 3/4, y + 1/4 [u, v, w]</td>
</tr>
<tr>
<td>(19) x + 1/4, z + 1/4, y + 3/4 [u, v, w]</td>
<td>(20) x + 3/4, z + 1/4, y + 3/4 [u, w, v]</td>
</tr>
<tr>
<td>(21) z + 1/4, y + 1/4, x + 1/4 [w, v, u]</td>
<td>(22) z + 3/4, y + 1/4, x + 1/4 [w, v, u]</td>
</tr>
<tr>
<td>(23) z + 3/4, y + 1/4, x + 3/4 [w, v, u]</td>
<td>(24) z + 1/4, y + 3/4, x + 3/4 [w, v, u]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1] p4gm'**
  - \( a^* = (a - b)/2 \)
  - \( b^* = (a + b)/2 \)

- **Along [1,1,1] p31m**
  - \( a^* = (2a - b - c)/3 \)
  - \( b^* = (-a + 2b - c)/3 \)

- **Along [1,1,0] \( c_{\alpha}p1m1 \)**
  - \( a^* = (-a + b)/2 \)
  - \( b^* = c/2 \)

**Origin at 0,1/4,z**

- **Origin at x,x,x**

**Origin at x,x+1/4,0**
Origin on 31' [1,1,1] at midpoint of three non-intersecting pairs of parallel 21' axes and of three non-intersecting pairs of parallel 211' axes

Asymmetric unit
\[ \frac{1}{4} \leq x \leq \frac{1}{2}; \quad \frac{1}{4} \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{2}; \quad z \leq \min(x,y) \]

Vertices

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/4,1/4,0</td>
<td>1/2,1/4,0</td>
<td>1/2,1/2,0</td>
</tr>
<tr>
<td>1/4,1/4,1/4</td>
<td>1/2,1/4,1/2</td>
<td>1/2,1/2,1/2</td>
</tr>
<tr>
<td>1/4,1/2,1/4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(2) 2 (0,0,1/2) 1/4,0,z
(2 | 1/2,0,1/2)

(3) 2 (0,1/2,0) 0,y,1/4
(2 | 0,1/2,1/2)

(4) 2 (1/2,0,0) x,1/4,0
(2 | 1/2,1/2,0)

(5) 3' x,x,x
(3 | 0,0,0)

(6) 3' \text{ x+1/2, x}, \text{x}
(3 | 1/2,1/2,0)

(7) 3' \text{x+1/2, x-1/2, x}
(3 | 1/2,0,1/2)

(8) 3' \text{ x, x+1/2, x}
(3 | 0,1/2,1/2)

(9) 3' x,x,x
(3 | 1/2,1/2,0)

(10) 3' \text{-1/3,1/3,1/3}
(3 | 0,1/2,1/2)

(11) 3' \text{1/3,1/-3,1/3}
(3 | 0,1/2,1/2)

(12) 3' \text{1/3,-1/3,1/3}
(3 | 0,1/2,1/2)

(13) d (1/4,1/4,1/4) x,x,z
(m | 1/4,1/4,1/4)

(14) d (-1/4,1/4,3/4) x+1/2, x,z
(m | 1/4,3/4,3/4)

(15) 4' \text{1/2,1/4,1/4}
(3 | 1/2,1/2,0)

(16) 4' \text{0,3/4,1/2; 0,3/4,1/2}
(4 | 3/4,1/2,1/2)

(17) d (1/4,1/4,1/4) x,y,y
(m | 1/4,1/4,1/4)

(18) 4' \text{x,1/-2,1/-4; 3/8,1/-2,1/-4}
(4 | 3/4,3/4,3/4)

(19) 4' \text{x,0,3/4; 1/8,0,3/4}
(4 | 3/4,3/4,3/4)

(20) d (3/4,-1/4,1/4) x,y+1/2, y
(m | 3/4,1/4,1/4)

(21) d (1/4,1/4,1/4) x,y,x
(m | 1/4,1/4,1/4)

(22) 4' \text{3/4,3/4,3/4}
(3 | 0,1/2,1/2)

(23) d (1/4,3/4,-1/4) x+1/2, y,x
(m | 3/4,3/4,3/4)

(24) 4' \text{-1/4,1/-4,1/-4; -1/4,3/8,1/-2}
(4 | 1/4,3/4,3/4)

For (1/2,1/2,1/2) + set

(1) t (1/2,1/2,1/2)
(1 | 1/2,1/2,1/2)

(2) 2 0,1/4,z
(2 | 1/2,0,1/2)

(3) 2 1/4,y,0
(2 | 1/2,0,1/2)

(4) 2 x,0,1/4
(2 | 0,1/2,1/2)

(5) 3' (1/2,1/2,1/2) x,x,x
(3 | 1/2,1/2,1/2)

(6) 3' (1/6,-1/6,1/6)
(3 | 0,0,1/2)

(7) 3' (-1/6,1/6,-1/6)
(3 | 0,1/2,2/0)

(8) 3' (1/6,1/6,-1/6)
(3 | 1/2,0,0)

(9) 3' (1/2,1/2,1/2) x,x,x
(3 | 1/2,1/2,1/2)

(10) 3' (1/6,-1/6,-1/6)
(3 | 0,1/2,1/2)

(11) 3' (-1/6,-1/6,-1/6)
(3 | 0,1/2,1/2)

(12) 3' (-1/6,1/6,-1/6)
(3 | 0,1/2,1/2)

(13) d (3/4,3/4,3/4) x,x,z
(m | 3/4,3/4,3/4)

(14) d (1/-4,1/-4,1/-4) x+1/2, x,z
(m | 1/4,3/4,3/4)

(15) 4' 1/2,1/4,1/4;
(4 | 1/4,3/4,3/4)

(16) 4' 0,1/4,z; 0,1/4,3/8
(4 | 1/4,1/4,3/4)

(17) d (3/4,3/4,3/4) x,y,y
(m | 3/4,3/4,3/4)

(18) 4' x,1/2,1/4; 1/8,1/2,1/4
(4 | 1/4,3/4,3/4)

(19) 4' x,0,1/4; 3/8,0,1/4
(4 | 1/4,1/4,3/4)

(20) d (1/4,1/4,-1/4) x,y+1/2, y
(m | 1/4,3/4,3/4)

(21) d (3/4,3/4,3/4) x,y,x
(m | 3/4,3/4,3/4)

(22) 4' 1/4,y,0; 1/4,0,3/8
(4 | 1/4,3/4,3/4)

(23) d (-1/4,1/4,1/4) x+1/2, y,x
(4 | 3/4,1/4,3/4)

(24) 4' 1/4,y,1/2; 1/4,1/8,1/2
(4 | 3/4,1/4,3/4)
Continued

For (0,0,0) + set

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,y,z</td>
<td>48</td>
</tr>
<tr>
<td>x+1/2,y+1/2,z+1/2</td>
<td>1/2</td>
</tr>
<tr>
<td>x,y+1/2,z+1/2</td>
<td>1/2</td>
</tr>
</tbody>
</table>

Generators selected

| (1) t (1/2,1/2,1/2) | (2) 2` (0,0,1/2) | (3) 2` (0,1,2,0) | (4) 2` (1,2,0,0) |

| Coordinates | (0,0,0) + (1/2,1/2,1/2) + (0,0,0)` + (1/2,1/2,1/2) + |

(1) x,y,z [0,0,0] (2) x+1/2,y+1/2,z+1/2 [0,0,0] (3) x,y+1/2,z+1/2 [0,0,0] (4) x+1/2,y+1/2,z+1/2 [0,0,0] (5) z,x,y [0,0,0] (6) z+1/2,x,y+1/2 [0,0,0] (7) z+1/2,x,y+1/2 [0,0,0] (8) z,x+1/2,y+1/2 [0,0,0]
Continued

(9) \( y,z,x \ [0,0,0] \)  

(10) \( y,z+1/2,x+1/2 \ [0,0,0] \)  

(11) \( y+1/2,z+1/2,x \ [0,0,0] \)  

(12) \( y+1/2,z,x+1/2 \ [0,0,0] \)  

(13) \( y+1/4,x+1/4,z+1/4 \ [0,0,0] \)  

(14) \( y+1/4,x+1/4,z+3/4,y+1/4 \ [0,0,0] \)  

(15) \( y+3/4,x+1/4,z+3/4 \ [0,0,0] \)  

(16) \( y+3/4,x+3/4,z+1/4 \ [0,0,0] \)  

(17) \( x+1/4,z+1/4,y+1/4 \ [0,0,0] \)  

(18) \( x+1/4,z+3/4,y+1/4 \ [0,0,0] \)  

(19) \( x+1/4,z+3/4,y+3/4 \ [0,0,0] \)  

(20) \( x+3/4,z+1/4,y+3/4 \ [0,0,0] \)  

(21) \( z+1/4,y+1/4,x+1/4 \ [0,0,0] \)  

(22) \( z+3/4,y+1/4,x+3/4 \ [0,0,0] \)  

(23) \( z+3/4,y+3/4,x+1/4 \ [0,0,0] \)  

(24) \( z+1/4,y+3/4,x+3/4 \ [0,0,0] \)  

24  d 2..1'  

\( x,0,1/4 \ [0,0,0] \)  

\( x+1/2,0,3/4 \ [0,0,0] \)  

1/4,x,0 [0,0,0]  

3/4,x+1/2,0 [0,0,0]  

0,1/4,x [0,0,0]  

0,3/4,x+1/2 [0,0,0]  

1/4,x+1/4,1/2 [0,0,0]  

1/4,x+3/4,0 [0,0,0]  

x+1/4,1/2,1/4 [0,0,0]  

\( x+3/4,0,1/4 \ [0,0,0] \)  

1/2,1/4,x+1/4 [0,0,0]  

0,1/4,x+3/4 [0,0,0]  

16  c 3..1'  

\( x,x \ [0,0,0] \)  

\( x+1/2,x \ [0,0,0] \)  

\( x+1/2,x+1/2 \ [0,0,0] \)  

\( x+1/2,x+1/2,x \ [0,0,0] \)  

\( x+1/4,x+1/4,x+1/4 \ [0,0,0] \)  

\( x+1/4,x+3/4,x+3/4 \ [0,0,0] \)  

\( x+3/4,x+1/4,x+3/4 \ [0,0,0] \)  

\( x+3/4,x+3/4,x+1/4 \ [0,0,0] \)  

12  b 41'  

\( 7/8,0,1/4 \ [0,0,0] \)  

\( 5/8,0,3/4 \ [0,0,0] \)  

1/4,7/8,0 [0,0,0]  

\( 3/4,5/8,0 \ [0,0,0] \)  

0,1/4,7/8 [0,0,0]  

0,3/4,5/8 [0,0,0]  

12  a 41'  

\( 3/8,0,1/4 \ [0,0,0] \)  

\( 1/8,0,3/4 \ [0,0,0] \)  

1/4,3/8,0 [0,0,0]  

\( 3/4,1/8,0 \ [0,0,0] \)  

0,1/4,3/8 [0,0,0]  

0,3/4,1/8 [0,0,0]  

\[ \text{Symmetry of Special Projections} \]  

\text{Along} [0,0,1] \quad \text{p4g}m1'  

\( a^* = (a - b)/2 \)  

\( b^* = (a + b)/2 \)  

\text{Origin at} 0,1/4,z  

\text{Along} [1,1,1] \quad \text{p31m}1'  

\( a^* = (2a - b - c)/3 \)  

\( b^* = (-a + 2b - c)/3 \)  

\text{Origin at} x,x,x  

\text{Along} [1,1,0] \quad \text{c1m}11'  

\( a^* = (a + b)/2 \)  

\( b^* = c/2 \)  

\text{Origin at} x,x+1/4,0
Origin on 3 [1,1,1] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 21 axes

Asymmetric unit

\[ \begin{align*}
1/4 \leq x & \leq 1/2; \\
1/4 \leq y & \leq 1/2; \\
0 \leq z & \leq 1/2; \\
z & \leq \text{min}(x,y)
\end{align*} \]

Vertices

\[ \begin{align*}
1/4,1/4,0 & \\
1/2,1/4,0 & \\
1/2,1/2,0 & \\
1/4,1/2,0 & \\
1/4,1/4,1/4 & \\
1/2,1/4,1/2 & \\
1/2,1/2,1/2 & \\
1/4,1/2,1/4
\end{align*} \]

Symmetry Operations

For (0,0,0) + set

\[ \begin{align*}
(1) & \quad 1 \\
(2) & \quad t(5/2,0,0); t(0,5/2,0); t(0,0,5/2); t(1/2,1/2,1/2); t(1,0,0,0)
\end{align*} \]

(5) \[3^+ x,x,x \]

\[ \begin{align*}
(6) & \quad 3^+ x+1/2,x,x \\
(3_{yz}) & \quad 1/2,1/2,0
\end{align*} \]

(9) \[3^- x,x,x \]

\[ \begin{align*}
(10) & \quad 3^+ x+1/2,x,x \quad x+1/6,x+1/6,x \\
(3_{yz})^- & \quad 1/2,1/2,0
\end{align*} \]

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13).
Continued 220.3.1593 14'3d'

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

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**Symmetry of Special Projections**

Origin at x,x,x

**Symmetry**

Along [0,0,1] p4g'm' 

Along [1,1,1] p31m' 

Along [1,1,0] c1m'1

**Origin at 0,1/4,z**

\( a^* = (a - b)/2 \) \( b^* = (a + b)/2 \)

\( a^* = (2a - b - c)/3 \) \( b^* = (-a + 2b - c)/3 \) \( a^* = (-a + b)/2 \) \( b^* = c/2 \)
Origin at center \((m\overline{3}m)\)

Asymmetric unit \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y\)

Vertices \(0,0,0\) \(1/2,0,0\) \(1/2,1/2,0\) \(1/2,1/2,1/2\)

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad (0,0,0) \\

(2) & \quad 2 \quad 0,0,z \\
(2) & \quad (0,0,0) \\

(3) & \quad 2 \quad 0, y, 0 \\
(3) & \quad (0,0,0) \\

(4) & \quad 2 \quad x, 0, 0 \\
(4) & \quad (0,0,0) \\

(5) & \quad 3^+ \quad x, x, x \\
(5) & \quad (3_{xyz} \, | \, 0,0,0) \\

(6) & \quad 3^- \quad x, x, x \\
(6) & \quad (3_{xyz}^{-1} \, | \, 0,0,0) \\

(7) & \quad 3^+ \quad x, x, x \\
(7) & \quad (3_{xyz} \, | \, 0,0,0) \\

(8) & \quad 3^- \quad x, x, x \\
(8) & \quad (3_{xyz}^{-1} \, | \, 0,0,0) \\

(9) & \quad 3^+ \quad x, x, x \\
(9) & \quad (3_{xyz} \, | \, 0,0,0) \\

(10) & \quad 3^- \quad x, x, x \\
(10) & \quad (3_{xyz}^{-1} \, | \, 0,0,0) \\

(11) & \quad 3^+ \quad x, x, x \\
(11) & \quad (3_{xyz} \, | \, 0,0,0) \\

(12) & \quad 3^- \quad x, x, x \\
(12) & \quad (3_{xyz}^{-1} \, | \, 0,0,0)
\end{align*}
\]
Continued 221.1.1594 Pm3m

(13) 2 x,x,0
(2) x,y,0
(14) 2 x,x,0
(2) x,y,0
(15) 4 y,0,z
(4) y,0,0
(16) 4 z,0,0
(4) z,0,0

(17) 4 y,0,0
(2) y,0,0
(18) 2 y,0,0
(2) y,0,0
(19) 2 y,0,0
(2) y,0,0

(21) 4 y,0,0
(2) y,0,0
(22) 2 x,0,x
(2) x,0,x
(23) 4 y,0,x
(2) y,0,x

(25) m 0,0,0
(1) m 0,0,0
(26) m x,x,0
(2) m x,x,0
(27) m x,0,z
(2) m x,0,z

(29) m x,x,x; 0,0,0
(3) m x,x,x; 0,0,0
(30) m x,x,x; 0,0,0
(3) m x,x,x; 0,0,0
(31) m x,x,x; 0,0,0
(3) m x,x,x; 0,0,0

(37) m x,x,z
(2) m x,x,z
(38) m x,x,z
(2) m x,x,z

(41) m x,x,0; 0,0,0
(2) m x,x,0; 0,0,0
(42) m x,x,0; 0,0,0
(2) m x,x,0; 0,0,0

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48 n 1

(1) x,y,z [u,v,w]
(2) y,z,x [u,v,w]
(3) x,y,z [u,v,w]
(4) x,z,y [u,v,w]
(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]
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(13) y,z,x [v,w,u]
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221.1.1594 - 2 - 3620
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<td>(40)</td>
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<td>$\bar{v} \cdot u \cdot w$</td>
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<td>$x \cdot z \cdot y$</td>
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<tr>
<td>1</td>
<td>a</td>
<td>m3m</td>
<td>0,0,0 [0,0,0]</td>
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</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1':  
\[ a^* = a \quad b^* = b \]

Origin at 0,0,z

Along [1,1,1] p6'm'm:  
\[ a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \]

Origin at x,x,x

Along [1,1,0] p2mm1':  
\[ a^* = (-a + b)/2 \quad b^* = c \]

Origin at x,x,0
Origin at center \((m\overline{3}m1')\)

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 1/2,1/2,1/2
\end{align*}
\]

Symmetry Operations

For 1 + set

\[
\begin{align*}
(1) & \quad 1 \quad (1|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \quad (2|0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \quad (2|0,0,0) \\
(4) & \quad 2 \quad x,0,0 \quad (2,|0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \quad (3_{xyz},|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \quad (3_{xyz},|0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \quad (3_{xyz},|0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \quad (3_{xyz},|0,0,0) \\
(9) & \quad 3^- \quad x,x,x \quad (3_{xyz},|0,0,0) \\
(10) & \quad 3^- \quad x,x,x \quad (3_{xyz},|0,0,0) \\
(11) & \quad 3^- \quad x,x,x \quad (3_{xyz},|0,0,0) \\
(12) & \quad 3^- \quad x,x,x \quad (3_{xyz},|0,0,0)
\end{align*}
\]
Continued

| 13 | 2' x,x,0 |
| 14 | 2' x,x,0 |
| 15 | 4' x,0,0 |
| 16 | 4' x,0,0 |

| 17 | 4' x,0,0 |
| 18 | 4' x,0,0 |
| 19 | 2 0,0 |
| 20 | 4' x,0,0 |

| 21 | 4' 0,0,0 |
| 22 | 4' 0,0,0 |
| 23 | 2 0,0 |
| 24 | 2 0,0,0 |

| 25 | 0,0,0 |
| 26 | 0,0,0 |
| 27 | 0,0,0 |
| 28 | 0,0,0 |

For 1' + set

| 1 | 1' |
| 2 | 1' |
| 3 | 2' |
| 4 | 2' |

| 5 | 3' x,x,x |
| 6 | 3' x,x,x |
| 7 | 3' x,x,x |
| 8 | 3' x,x,x |

| 9 | 3' x,x,x |
| 10 | 3' x,x,x |
| 11 | 3' x,x,x |
| 12 | 3' x,x,x |

| 13 | 2' x,x,0 |
| 14 | 2' x,x,0 |
| 15 | 2' x,x,0 |
| 16 | 2' x,x,0 |

| 17 | 4' x,0,0 |
| 18 | 4' x,0,0 |
| 19 | 4' x,0,0 |
| 20 | 4' x,0,0 |

| 21 | 4' 0,0,0 |
| 22 | 4' 0,0,0 |
| 23 | 4' 0,0,0 |
| 24 | 4' 0,0,0 |

| 25 | 0,0,0 |
| 26 | 0,0,0 |
| 27 | 0,0,0 |
| 28 | 0,0,0 |

| 29 | 3' x,x,x |
| 30 | 3' x,x,x |
| 31 | 3' x,x,x |
| 32 | 3' x,x,x |

| 33 | 3' x,x,x |
| 34 | 3' x,x,x |
| 35 | 3' x,x,x |
| 36 | 3' x,x,x |

| 221.2.1595 | Pm3m1' |
### Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25); 1'.

### Positions

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<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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<td>(2) x,y,z [0,0,0]</td>
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221.2.1595 - 3 - 3625
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<tr>
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<td>3 d 4/mm.m1'</td>
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</table>
1  b  \(m\overline{3}m1'\) 1/2,1/2,1/2 [0,0,0]
1  a  \(m\overline{3}m1'\) 0,0,0 [0,0,0]

**Symmetry of Special Projections**

Along [0,0,1]  p4mm1'
\[a^* = a\quad b^* = b\]
Origin at 0,0,z

Along [1,1,1]  p6mm1'
\[a^* = (2a - b - c)/3\quad b^* = (-a + 2b - c)/3\]
Origin at x,x,x

Along [1,1,0]  p2mm1'
\[a^* = (-a + b)/2\quad b^* = c\]
Origin at x,x,0
Origin at center (m'3'm)

Asymmetric unit

0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ x; z ≤ y

Vertices

0,0,0 1/2,0,0 1/2,1/2,0 1/2,1/2,1/2

Symmetry Operations

1

(1) 1
(2) 2 0,0,z
(2z | 0,0,0)
(3) 2 0,y,0
(2y | 0,0,0)
(4) 2 x,0,0
(2x | 0,0,0)

(5) 3' x,x,x
(3xyz | 0,0,0)
(6) 3' x,x,x
(3xyz⁻¹ | 0,0,0)
(7) 3' x,x,x
(3xyz⁻¹ | 0,0,0)
(8) 3' x,x,x
(3xyz⁻¹ | 0,0,0)

(9) 3' x,x,x
(3xyz⁻¹ | 0,0,0)
(10) 3' x,x,x
(3xyz⁻¹ | 0,0,0)
(11) 3' x,x,x
(3xyz⁻¹ | 0,0,0)
(12) 3' x,x,x
(3xyz⁻¹ | 0,0,0)
Continued

| (13) 2' x,x,0 | (14) 2' x,x,0 | (15) 4' 0,0,z | (16) 4' 0,0,z |
| (2y, 0,0,0)' | (2y, 0,0,0)' | (4z, 0,0,0)' | (4z, 0,0,0)' |
| (17) 4' x,0,0 | (18) 2' 0,y,y | (19) 2' 0,y,y | (20) 4' x,0,0 |
| (4z' 1,0,0)' | (2y, 0,0,0)' | (2y, 0,0,0)' | (4z, 0,0,0)' |
| (21) 4' 0,y,0 | (22) 2' x,0,x | (23) 4' 0,y,0 | (24) 2' x,0,x |
| (4y, 0,0,0)' | (2x, 0,0,0)' | (4y, 0,0,0)' | (2zx, 0,0,0)' |
| (25) 1' 0,0,0 | (26) m' x,y,0 | (27) m' x,0,z | (28) m' 0,y,0 |
| (1', 0,0,0)' | (mxy, 0,0,0)' | (mxy, 0,0,0)' | (mxy, 0,0,0)' |
| (29) 3' x,x,x; 0,0,0 | (30) 3' x,x,x; 0,0,0 | (31) 3' x,x,x; 0,0,0 | (32) 3' x,x,x; 0,0,0 |
| (3xyz, 0,0,0)' | (3xyz, 0,0,0)' | (3xyz, 0,0,0)' | (3xyz, 0,0,0)' |
| (33) 3' x,x,x; 0,0,0 | (34) 3' x,x,x; 0,0,0 | (35) 3' x,x,x; 0,0,0 | (36) 3' x,x,x; 0,0,0 |
| (3xyz, 0,0,0)' | (3xyz, 0,0,0)' | (3xyz, 0,0,0)' | (3xyz, 0,0,0)' |
| (37) m x,x,z | (38) m x,x,z | (39) 4' 0,0,z; 0,0,0 | (40) 4' 0,0,z; 0,0,0 |
| (mxyz, 0,0,0) | (mxyz, 0,0,0) | (mxyz, 0,0,0) | (mxyz, 0,0,0) |
| (41) 4' x,0,0; 0,0,0 | (42) m x,y,y | (43) m x,y,y | (44) 4' x,0,0; 0,0,0 |
| (4y, 0,0,0)' | (mxy, 0,0,0) | (mxy, 0,0,0) | (4y, 0,0,0) |
| (45) 4' 0,y,0; 0,0,0 | (46) m x,y,x | (47) 4' 0,y,0; 0,0,0 | (48) m x,y,x |
| (4y, 0,0,0)' | (mxyz, 0,0,0) | (mxyz, 0,0,0) | (mxyz, 0,0,0) |

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

Positions

Multiplicity
Wyckoff letter
Site Symmetry.

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<td>(2) x,y,z [u,v,w]</td>
<td>(3) x,y,z [u,v,w]</td>
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<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) z,x,y [w,u,v]</td>
<td>(7) z,x,y [w,u,v]</td>
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<td>(9) y,z,x [v,w,u]</td>
<td>(10) y,z,x [v,w,u]</td>
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221.3.1596 - 2 - 3629
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<td>(38) $y, x, z [v, u, w]$</td>
<td>$x, x, z [u, u, 0]$</td>
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<td>(39) $\overline{y}, x, z [v, u, w]$</td>
<td>$x, x, z [u, u, 0]$</td>
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<td>(40) $y, x, z [v, u, w]$</td>
<td>$x, x, z [u, u, 0]$</td>
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<tr>
<td>(41) $\overline{x}, z, y [u, w, v]$</td>
<td>24 l..m $1/2, y, z [0, v, w]$</td>
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<tr>
<td>(42) $\overline{x}, z, y [u, w, v]$</td>
<td>$1/2, y, z [0, v, w]$</td>
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<td>(43) $x, z, y [u, w, v]$</td>
<td>$1/2, y, z [0, v, w]$</td>
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<td>(44) $\overline{x}, z, y [u, w, v]$</td>
<td>$1/2, y, z [0, v, w]$</td>
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<tr>
<td>(45) $\overline{z}, y, x [w, v, u]$</td>
<td>24 k..m $0, y, z [0, v, w]$</td>
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<tr>
<td>(46) $\overline{z}, y, x [w, v, u]$</td>
<td>$0, y, z [0, v, w]$</td>
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<tr>
<td>(47) $z, y, x [w, v, u]$</td>
<td>$0, y, z [0, v, w]$</td>
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<td>$0, y, z [0, v, w]$</td>
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<tr>
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<td>12 j..m $1/2, y, y [u, u, v]$</td>
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<tr>
<td>(56) $y, 1/2, z [v, 0, w]$</td>
<td>$1/2, y, y [u, u, v]$</td>
</tr>
<tr>
<td>(57) $y, 1/2, z [v, 0, w]$</td>
<td>$1/2, y, y [u, u, v]$</td>
</tr>
<tr>
<td>(58) $y, 1/2, z [v, 0, w]$</td>
<td>$1/2, y, y [u, u, v]$</td>
</tr>
<tr>
<td>(59) $y, 1/2, z [v, 0, w]$</td>
<td>$1/2, y, y [u, u, v]$</td>
</tr>
<tr>
<td>12</td>
<td>h</td>
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<tr>
<td>----</td>
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</tr>
<tr>
<td></td>
<td>1/2,0,x [0,0,u]</td>
</tr>
<tr>
<td></td>
<td>(x,0,1/2 [\bar{u},0,0])</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
</tr>
<tr>
<td></td>
<td>(x,0,0) [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>f</td>
</tr>
<tr>
<td></td>
<td>(1/2,\bar{x},1/2 [0,0,0])</td>
</tr>
<tr>
<td>6</td>
<td>e</td>
</tr>
<tr>
<td></td>
<td>(0,\bar{x},0 [0,0,0])</td>
</tr>
<tr>
<td>3</td>
<td>d</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along \([0,0,1]\)**: \(p4'm'm\)  
  \(a^* = a\)  \(b^* = b\)  
  Origin at 0,0,z

- **Along \([1,1,1]\)**: \(p6mm\)  
  \(a^* = (2a - b - c)/3\)  \(b^* = (-a + 2b - c)/3\)  
  Origin at x,x,x

- **Along \([1,1,0]\)**: \(p2mm1'\)  
  \(a^* = (-a + b)/2\)  \(b^* = c\)  
  Origin at x,x,0
**Origin** at center (m\(\overline{3}\)m')

**Asymmetric unit**

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y\]

**Vertices**

- 0,0,0
- 1/2,0,0
- 1/2,1/2,0
- 1/2,1/2,1/2

**Symmetry Operations**

1. \(1\)
   - (1) \(1\)
   - (2) \(2, 0, 0, 0\)
   - (3) \(2, 0, y, 0\)
   - (4) \(2, x, 0, 0\)
2. \(3\)
   - (5) \(3^+, x, x, x\)
   - (6) \(3^+, x, x, x\)
   - (7) \(3^+, x, x, x\)
   - (8) \(3^+, x, x, x\)
3. \(3\)
   - (9) \(3^-, x, x, x\)
   - (10) \(3^-, x, x, x\)
   - (11) \(3^-, x, x, x\)
   - (12) \(3^-, x, x, x\)
Continued

Generators selected \( (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25). \)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

\[
\begin{array}{cccc}
48 & n & 1 & \\
(1) & x,y,z & [u,v,w] & (2) \bar{x},\bar{y},\bar{z} & [\bar{u},\bar{v},\bar{w}] & (3) \bar{x},y,\bar{z} & [\bar{u},v,w] & (4) x,\bar{y},\bar{z} & [u,\bar{v},\bar{w}] \\
(5) & z,x,y & [w,u,v] & (6) \bar{z},\bar{x},y & [\bar{w},u,\bar{v}] & (7) \bar{z},x,\bar{y} & [w,\bar{u},\bar{v}] & (8) \bar{z},x,y & [w,u,\bar{v}] \\
(9) & y,z,x & [v,w,u] & (10) \bar{y},\bar{z},x & [\bar{v},w,\bar{u}] & (11) \bar{y},z,\bar{x} & [\bar{v},w,\bar{u}] & (12) \bar{y},z,x & [\bar{v},w,\bar{u}] \\
(13) & y,x,z & [\bar{v},\bar{u},w] & (14) \bar{y},\bar{x},\bar{z} & [\bar{v},\bar{u},w] & (15) \bar{y},x,z & [\bar{v},u,\bar{w}] & (16) \bar{y},x,z & [\bar{v},u,\bar{w}] \\
(17) & x,z,y & [\bar{u},\bar{w},v] & (18) \bar{x},\bar{z},y & [\bar{u},\bar{w},v] & (19) \bar{x},z,\bar{y} & [u,\bar{w},\bar{v}] & (20) \bar{x},z,y & [u,\bar{w},\bar{v}] \\
(21) & z,y,x & [w,\bar{v},u] & (22) \bar{z},\bar{y},x & [\bar{w},\bar{v},u] & (23) \bar{z},y,\bar{x} & [w,\bar{v},\bar{u}] & (24) \bar{z},y,\bar{x} & [w,\bar{v},\bar{u}] \\
(25) & \bar{x},y,\bar{z} & [u,v,w] & (26) x,y,\bar{z} & [v,\bar{u},w] & (27) x,\bar{y},z & [u,v,\bar{w}] & (28) x,\bar{y},z & [u,v,\bar{w}] \\
(29) & z,\bar{x},y & [w,\bar{u},v] & (30) \bar{z},x,y & [\bar{w},u,\bar{v}] & (31) \bar{z},x,\bar{y} & [w,u,\bar{v}] & (32) \bar{z},x,y & [w,u,\bar{v}] \\
(33) & \bar{y},z,\bar{x} & [v,\bar{w},u] & (34) y,z,\bar{x} & [v,\bar{w},u] & (35) y,\bar{z},x & [v,\bar{w},u] & (36) y,\bar{z},x & [v,\bar{w},u] \\
\end{array}
\]
<table>
<thead>
<tr>
<th>12</th>
<th>h</th>
<th>mm2..</th>
<th>x,1/2,0 [0,0,0]</th>
<th>x,1/2,0 [0,0,0]</th>
<th>0,x,1/2 [0,0,0]</th>
<th>0,x,1/2 [0,0,0]</th>
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<tbody>
<tr>
<td></td>
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<td>1/2,0,x [0,0,0]</td>
<td>1/2,0,x [0,0,0]</td>
<td>1/2,x,0 [0,0,0]</td>
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<td>x,0,1/2 [0,0,0]</td>
<td>x,0,1/2 [0,0,0]</td>
<td>0,1/2,x [0,0,0]</td>
<td>0,1/2,x [0,0,0]</td>
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<tr>
<td>8</td>
<td>g</td>
<td>.3m'</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
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<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
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<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
</tr>
<tr>
<td>6</td>
<td>f</td>
<td>4'm.m'</td>
<td>x,1/2,1/2 [0,0,0]</td>
<td>x,1/2,1/2 [0,0,0]</td>
<td>1/2,x,1/2 [0,0,0]</td>
<td>1/2,x,1/2 [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>1/2,x,1/2 [0,0,0]</td>
<td>1/2,x,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,x [0,0,0]</td>
<td>1/2,1/2,x [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>e</td>
<td>4'm.m'</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
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<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>d</td>
<td>4'/mm.m'</td>
<td>1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>3</td>
<td>c</td>
<td>4'/mm.m'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>b</td>
<td>m3m'</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>1</td>
<td>a</td>
<td>m3m'</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'
\[ a^* = a \quad b^* = b \]
Origin at 0,0,z

Along [1,1,1] p6'mm'
\[ a^* = (2a - b - c)/3 \quad b^* = (-a + 2b - c)/3 \]
Origin at x,x,x

Along [1,1,0] p2'mm'
\[ a^* = c \quad b^* = (-a + b)/2 \]
Origin at x,x,0
Origin at center \(m'3'm'\)

Asymmetric unit

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y
\]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 1/2,1/2,1/2 \\
\end{align*}
\]

Symmetry Operations

\[
\begin{align*}
(1) & \quad 1 & \quad (1|0,0,0) \\
(2) & \quad 2 & \quad 0,0,0, \quad (2_z|0,0,0) \\
(3) & \quad 2 & \quad 0,y,0, \quad (2_y|0,0,0) \\
(4) & \quad 2 & \quad x,0,0, \quad (2_x|0,0,0) \\
(5) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}^{-1}|0,0,0) \\
(7) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}^{-1}|0,0,0) \\
(8) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}^{-1}|0,0,0) \\
(9) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}|0,0,0) \\
(10) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}|0,0,0) \\
(11) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}|0,0,0) \\
(12) & \quad 3^+ & \quad x,x,x, \quad (3_{xyz}|0,0,0) \\
\end{align*}
\]
Continued

Wyckoff letter, Multiplicity, Positions

Continued 221.5.1598

48 n 1

Generators selected (1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

Positions

221.5.1598

221.5.1598 - 2 - 3637
Continued

<table>
<thead>
<tr>
<th>12</th>
<th>h</th>
<th>m'm'2.. x,1/2,0 [u,0,0]</th>
<th>x,1/2,0 [u,0,0]</th>
<th>0,x,1/2 [0,u,0]</th>
<th>0,x,1/2 [0,u,0]</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
<td>1/2,0,x [0,0,u]</td>
<td>1/2,0,x [0,0,u]</td>
<td>1/2,x,0 [0,u,0]</td>
<td>1/2,x,0 [0,u,0]</td>
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<tr>
<td></td>
<td></td>
<td>x,0,1/2 [u,0,0]</td>
<td>x,0,1/2 [u,0,0]</td>
<td>0,1/2,x [0,0,u]</td>
<td>0,1/2,x [0,0,u]</td>
</tr>
<tr>
<td>8</td>
<td>g</td>
<td>.3m' x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6 f 4m'.m' x,1/2,1/2 [u,0,0]</td>
<td>x,1/2,1/2 [u,0,0]</td>
<td>1/2,x,1/2 [0,u,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/2,x,1/2 [0,u,0]</td>
<td>1/2,1/2,x [0,0,u]</td>
<td>1/2,1/2,x [0,0,u]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6 e 4m'.m' x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [0,u,0]</td>
<td>0,x,0 [0,u,0]</td>
</tr>
<tr>
<td></td>
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<td>0,x,0 [0,u,0]</td>
<td>0,0,x [0,0,u]</td>
<td>0,0,x [0,0,u]</td>
<td>0,0,x [0,0,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3 d 4/m'm'.m' 1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3 c 4/m'm'.m' 0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 b m'3m' 1/2,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 a m'3m' 0,0,0 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4m'm'</th>
<th>a⁺ = a</th>
<th>b⁺ = b</th>
<th>Origin at 0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>a⁺ = a</td>
<td>b⁺ = b</td>
<td>Origin at x,x,x</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,1]</th>
<th>p6m'm'</th>
<th>a⁺ = (2a - b - c)/3</th>
<th>b⁺ = (-2b + c)/3</th>
<th>Origin at x,x,0</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
<th>a⁺ = (-a + b)/2</th>
<th>b⁺ = c</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Origin at x,x,0</td>
<td></td>
</tr>
</tbody>
</table>
**Origin** at center (m\(\overline{3}\)m)

**Asymmetric unit**  

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y\]

**Vertices**  

\[0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/2,1/2,1/2\]

**Symmetry Operations**

For \((0,0,0)\) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>((1</td>
</tr>
<tr>
<td>2</td>
<td>((2</td>
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<tr>
<td>3</td>
<td>((3</td>
</tr>
<tr>
<td>4</td>
<td>((4</td>
</tr>
</tbody>
</table>

\[\begin{align*}
(5) \quad &3^+ \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(6) \quad &3^+ \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(7) \quad &3^+ \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(8) \quad &3^+ \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(9) \quad &3^- \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(10) \quad &3^- \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(11) \quad &3^- \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(12) \quad &3^- \quad x,x,x \\
&\quad \left(\begin{smallmatrix} x \quad x \quad x \\
\quad \end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(13) \quad &2 \quad x,x,0
\end{align*}\]

\[\begin{align*}
(14) \quad &2 \quad x,x,0
\end{align*}\]

\[\begin{align*}
(15) \quad &4^- \quad 0,0,z
\end{align*}\]

\[\begin{align*}
(16) \quad &4^- \quad 0,0,z
\end{align*}\]

\[\begin{align*}
(17) \quad &4^- \quad 0,y,0
\end{align*}\]

\[\begin{align*}
(18) \quad &2 \quad 0,y,y
\end{align*}\]

\[\begin{align*}
(19) \quad &2 \quad 0,y,y
\end{align*}\]

\[\begin{align*}
(20) \quad &4^- \quad x,0,0
\end{align*}\]

\[\begin{align*}
(21) \quad &4^- \quad 0,y,0
\end{align*}\]

\[\begin{align*}
(22) \quad &2 \quad x,0,x
\end{align*}\]

\[\begin{align*}
(23) \quad &4^- \quad y,0,0
\end{align*}\]

\[\begin{align*}
(24) \quad &2 \quad x,0,x
\end{align*}\]

\[\begin{align*}
(25) \quad &\overline{1} \quad 0,0,0
\end{align*}\]

\[\begin{align*}
(26) \quad &m \quad x,y,0
\end{align*}\]

\[\begin{align*}
(27) \quad &m \quad x,0,z
\end{align*}\]

\[\begin{align*}
(28) \quad &m \quad 0,y,z
\end{align*}\]

\[\begin{align*}
(29) \quad &3^+ \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(30) \quad &3^+ \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(31) \quad &3^+ \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(32) \quad &3^+ \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(33) \quad &3^- \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(34) \quad &3^- \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(35) \quad &3^- \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(36) \quad &3^- \quad x,x,x;0,0,0
\end{align*}\]

\[\begin{align*}
(37) \quad &m \quad x,x,z
\end{align*}\]

\[\begin{align*}
(38) \quad &m \quad x,x,z
\end{align*}\]

\[\begin{align*}
(39) \quad &4^- \quad 0,0,z;0,0,0
\end{align*}\]

\[\begin{align*}
(40) \quad &4^- \quad 0,0,z;0,0,0
\end{align*}\]

\[\begin{align*}
(41) \quad &4^- \quad 0,0,0;0,0,0
\end{align*}\]

\[\begin{align*}
(42) \quad &m \quad x,y,y
\end{align*}\]

\[\begin{align*}
(43) \quad &m \quad x,y,y
\end{align*}\]

\[\begin{align*}
(44) \quad &4^- \quad x,0,0;0,0,0
\end{align*}\]

\[\begin{align*}
(45) \quad &4^- \quad 0,y,0;0,0,0
\end{align*}\]

\[\begin{align*}
(46) \quad &m \quad x,y,x
\end{align*}\]

\[\begin{align*}
(47) \quad &4^- \quad y,0,0;0,0,0
\end{align*}\]

\[\begin{align*}
(48) \quad &m \quad x,y,x
\end{align*}\]

**For \((1,0,0)^\prime\) + set**

<table>
<thead>
<tr>
<th>No.</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>((1</td>
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<tr>
<td>2</td>
<td>((2</td>
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<tr>
<td>3</td>
<td>((3</td>
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<tr>
<td>4</td>
<td>((4</td>
</tr>
</tbody>
</table>

\[\begin{align*}
(5) \quad &3^- \quad \left(\begin{smallmatrix} 1/3,1/3,1/3 \\
+2/3,x+1/3,x \\
(3_{xyz}|1,0,0)^\prime
\end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(6) \quad &3^- \quad \left(\begin{smallmatrix} 1/3,1/3,1/3 \\
+2/3,x+1/3,x \\
(3_{xyz}|1,0,0)^\prime
\end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(7) \quad &3^- \quad \left(\begin{smallmatrix} 1/3,1/3,1/3 \\
+2/3,x+1/3,x \\
(3_{xyz}|1,0,0)^\prime
\end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(8) \quad &3^- \quad \left(\begin{smallmatrix} 1/3,1/3,1/3 \\
+2/3,x+1/3,x \\
(3_{xyz}|1,0,0)^\prime
\end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(9) \quad &3^- \quad \left(\begin{smallmatrix} 1/3,1/3,1/3 \\
+2/3,x+1/3,x \\
(3_{xyz}|1,0,0)^\prime
\end{smallmatrix}\right)
\end{align*}\]

\[\begin{align*}
(10) \quad &3^- \quad \left(\begin{smallmatrix} 1/3,1/3,1/3 \\
+2/3,x+1/3,x \\
(3_{xyz}|1,0,0)^\prime
\end{smallmatrix}\right)
\end{align*}\]
Continued 221.6.1599 P $\bar{m}$3m

\[
\begin{array}{ll}
(13) & 2' (1/2,1/2,0) \ x+1,x+1/2,0 \\
(14) & 2' (-1/2,1/2,0) \ x+1,x-1/2,0 \\
(15) & 4' \ 1/2,-1/2,z \\
(16) & 4' \ 1/2,1/2,z \\
(17) & 4' \ (1,0,0) \ x,0,0 \\
(18) & 2' \ 1/2,y,y \\
(19) & 2' \ 1/2,y,-y \\
(20) & 2' (1,0,0) \ x,0,0 \\
(21) & 4' \ 1/2,y,-1/2 \\
(22) & 2' \ (1/2,0,1/2) \ x+1/2,0,x \\
(23) & 4' \ 1/2,y,1/2 \\
(24) & 2' \ x+1/2,0,x \\
(25) & \bar{1} \ 1/2,0,0 \\
(26) & a' (1,0,0) \ x,y,0 \\
(27) & a' (1,0,0) \ x,0,z \\
(28) & m' \ 1/2,y,z \\
(29) & 3' \ x,x-1,x; \\
(30) & 3' \ x,x+1/2,x; \\
(31) & 3' \ x,x+1,x; \\
(32) & 3' \ x,x+1,x; \\
(33) & 3' \ x+1,x+1,x; \\
(34) & 3' \ x+1,x-1,x; \\
(35) & 3' \ x+1,x,1; \\
(36) & 3' \ x+1,x-1,x; \\
(37) & g'(1/2,-1/2,0) \ x+1/2,x,z \\
(38) & g'(1/2,1/2,0) \ x+1/2,x,z \\
(39) & g' \ 1/2,1/2,z; 1/2,1/2,0 \\
(40) & g' \ 1/2,1/2,z; 1/2,1/2,0 \\
(41) & 4' \ x+1,0,0; 1/2,0,0 \\
(42) & a' (1,0,0) \ x,y,y \\
(43) & a' (1,0,0) \ x,y,y \\
(44) & 4' \ x+1,0,0; 1/2,0,0 \\
(45) & 4' \ 1/2,0,1/2; 1/2,0,1/2 \\
(46) & g'(1/2,0,1/2) \ x+1/2,y,x \\
(47) & g' \ 1/2,0,1/2; 1/2,0,-1/2 \\
(48) & g' \ 1/2,0,1/2) \ x+1/2,y,x \\
\end{array}
\]

Generators selected (1); t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13); (25).

**Positions**

<table>
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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>96</td>
<td>n 1</td>
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</tbody>
</table>

\[
(0,0,0) + (1,0,0)'
\]

\[
\begin{array}{ll}
(1) & x,y,z \ [u,v,w] \\
(2) & \bar{x},\bar{y},z \ [\bar{u},\bar{v},w] \\
(3) & \bar{x},y,z \ [\bar{u},v,w] \\
(4) & x,y,z \ [u,v,w] \\
(5) & z,x,y \ [w,u,v] \\
(6) & z,x,y \ [w,u,v] \\
(7) & \bar{z},x,y \ [w,u,v] \\
(8) & \bar{z},x,y \ [w,u,v] \\
(9) & y,z,x \ [v,w,u] \\
(10) & y,z,x \ [v,w,u] \\
(11) & y,z,x \ [v,w,u] \\
(12) & \bar{y},z,x \ [\bar{v},\bar{w},u] \\
(13) & y,x,z \ [v,u,w] \\
(14) & y,x,z \ [v,u,w] \\
(15) & y,x,z \ [v,u,w] \\
(16) & \bar{y},x,z \ [\bar{v},u,w] \\
(17) & x,z,y \ [u,w,\bar{v}] \\
(18) & x,z,y \ [u,w,\bar{v}] \\
(19) & x,z,y \ [u,w,\bar{v}] \\
(20) & x,z,y \ [u,w,\bar{v}] \\
(21) & z,y,x \ [w,v,u] \\
(22) & z,y,x \ [w,v,u] \\
(23) & z,y,x \ [w,v,u] \\
(24) & z,y,x \ [w,v,u] \\
(25) & x,y,z \ [u,v,w] \\
(26) & x,y,z \ [u,v,w] \\
(27) & x,y,z \ [u,v,w] \\
(28) & x,y,z \ [u,v,w] \\
(29) & z,x,y \ [w,u,v] \\
(30) & z,x,y \ [w,u,v] \\
(31) & z,x,y \ [w,u,v] \\
(32) & z,x,y \ [w,u,v] \\
(33) & \bar{y},z,x \ [v,w,u] \\
(34) & y,z,x \ [v,w,u] \\
(35) & \bar{y},z,x \ [\bar{v},w,u] \\
(36) & y,z,x \ [v,w,u] \\
\end{array}
\]
| (37) \( \bar{y}, x, z \) [\( v, u, w \)] | (38) \( y, x, z \) [\( v, u, w \)] | (39) \( y, x, z \) [\( v, u, w \)] | (40) \( y, x, z \) [\( v, u, w \)] |
| (41) \( x, z, y \) [\( u, w, v \)] | (42) \( x, z, y \) [\( u, w, v \)] | (43) \( x, y, z \) [\( u, w, v \)] | (44) \( x, z, y \) [\( u, w, v \)] |
| (45) \( z, y, x \) [\( w, v, u \)] | (46) \( z, y, x \) [\( w, v, u \)] | (47) \( z, y, x \) [\( w, v, u \)] | (48) \( z, y, x \) [\( w, v, u \)] |

<p>| 48 m | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] |
| 48 l | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] |
| 48 k | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] |
| 24 j | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] |
| 24 i | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] | 1/2, y, z [( 0, v, w )] |</p>
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<td>1/2,0, x [0, w,0]</td>
<td>1/2,x,0 [0,0,w]</td>
<td>1/2,x,0 [0,0,w]</td>
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<td>x,0,1/2 [0,w,0]</td>
<td>0,1/2, x [w,0,0]</td>
<td>0,1/2, x [w,0,0]</td>
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<td>x,1/2,1/2 [0,0,0]</td>
<td>x,1/2,1/2 [0,0,0]</td>
<td>1/2,x,1/2 [0,0,0]</td>
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<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
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<tr>
<td>6</td>
<td>d</td>
<td>4/m'm.m</td>
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<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
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<tr>
<td>6</td>
<td>c</td>
<td>4'/mm'.m</td>
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<td>1/2,0,1/2 [0,0,0]</td>
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<th>1/2,1/2,1/2 [0,0,0]</th>
<th>1/2,1/2,1/2 [0,0,0]</th>
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<tr>
<td>2</td>
<td>a</td>
<td>m3m</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
<td>0,0,0 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
\( a^* = a \)  \( b^* = b \)  
Origin at 0,0,z

Along [1,1,1] p6mm1'  
\( a^* = (2a - b - c)/3 \)  \( b^* = (-a + 2b - c)/3 \)  
Origin at x,x,x

Along [1,1,0] p2mm1'  
\( a^* = (-a + b)/2 \)  \( b^* = c \)  
Origin at x,x,0
Origin at center (m\overline{3}m')

Asymmetric unit: 0 < x ≤ 1/2; 0 < y ≤ 1/2; 0 < z ≤ 1/2; 0 < y; z ≤ y

Vertices: (0,0,0) 1/2,0,0 1/2,1/2,0 1/2,1/2,1/2

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)
(2) 2 0,0,z
(2z | 0,0,0)
(3) 2 0,y,0
(2y | 0,0,0)
(4) 2 x,0,0
(2x | 0,0,0)
(5) 3' x,x,x
(3xyz | 0,0,0)
(6) 3' \bar{x},x,\bar{x}
(3xyz-1 | 0,0,0)
(7) 3' x,\bar{x},x
(3xyz | 0,0,0)
(8) 3' \bar{x},x,\bar{x}
(3xyz-1 | 0,0,0)
(9) 3' x,x,x
(3xyz | 0,0,0)
(10) 3' \bar{x},\bar{x},\bar{x}
(3xyz-1 | 0,0,0)
(11) 3' \bar{x},x,x
(3xyz | 0,0,0)
(12) 3' x,\bar{x},\bar{x}
(3xyz-1 | 0,0,0)
(13) 2' x,x,0
(2xy | 0,0,0)'
(14) 2' \bar{x},x,0
(2xy | 0,0,0)'
(15) 4' 0,0,z
(4z | 0,0,0)'
(16) 4' 0,0,z
(4z | 0,0,0)'
(17) 4' x,0,0
(4x | 0,0,0)'
(18) 2' x,0,y
(2xy | 0,0,0)'
(19) 2' \bar{x},0,y
(2xy | 0,0,0)'
(20) 4' x,0,0
(4x | 0,0,0)'
(21) 4' x,0,0
(4x | 0,0,0)'
(22) 2' \bar{x},z,0
(2xz | 0,0,0)'
(23) 4' \bar{x},z,0
(2xz | 0,0,0)'
(24) 2' \bar{x},0,x
(2xz | 0,0,0)'
(25) 1 0,0,0
(1 | 0,0,0)
(26) m x,0,y
(my | 0,0,0)
(27) m x,0,z
(mz | 0,0,0)
(28) m y,z
(mz | 0,0,0)
(29) 3' x,x,x; 0,0,0
(3xyz | 0,0,0)
(30) 3' \bar{x},\bar{x},\bar{x}; 0,0,0
(3xyz-1 | 0,0,0)
(31) 3' \bar{x},\bar{x},x; 0,0,0
(3xyz | 0,0,0)
(32) 3' \bar{x},\bar{x},x; 0,0,0
(3xyz-1 | 0,0,0)
(33) m' x,x,z
(mx | 0,0,0)'
(34) m' x,x,\bar{z}
(mx | 0,0,0)'
(35) m' x,\bar{x},x
(mx | 0,0,0)'
(36) m' x,\bar{x},x
(mx | 0,0,0)'
(37) m' x,x,z
(mx | 0,0,0)'
(38) m' x,x,\bar{z}
(mx | 0,0,0)'
(39) 4' 0,0,z; 0,0,0
(4z | 0,0,0)'
(40) 4' 0,0,z; 0,0,0
(4z | 0,0,0)'
(41) 4' x,0,0; 0,0,0
(4x | 0,0,0)'
(42) m' x,y,y
(my | 0,0,0)'
(43) m' x,y,y
(my | 0,0,0)'
(44) 4' x,0,0; 0,0,0
(4x | 0,0,0)'
(45) 4' x,0,0; 0,0,0
(4x | 0,0,0)'

For (1,0,0)'+ set

(1) t' (1,0,0)
(1 | 1,0,0)'
(2) 2' 1/2,0,z
(2z | 1,0,0)'
(2) 2' 1/2,0,z
(2z | 1,0,0)'
(4) 2' (1,0,0) x,0,0
(2 | 1,0,0)'
(5) 3' (1/3,1/3,1/3)
(3xyz | 1,0,0)'
(6) 3' (1/3,-1/3,1/3)
(3xyz | 1,0,0)'
(7) 3' (1/3,-1/3,-1/3)
(3xyz-1 | 1,0,0)'
(8) 3' (1/3,1/3,1/3)
(3xyz-1 | 1,0,0)'
(9) 3' (1/3,1/3,-1/3)
(3xyz | 1,0,0)'
(10) 3' (1/3,-1/3,1/3)
(3xyz | 1,0,0)'
(11) 3' (1/3,1/3,-1/3)
(3xyz | 1,0,0)'
(12) 3' (1/3,-1/3,1/3)
(3xyz | 1,0,0)'

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(13) $2 \cdot (1/2,1/2,0) \ x+1, x+1/2, 0$

(2) $y + z \cdot (u, v, w)$

(14) $2 \cdot (-1/2,1/2,0) \ x+1, -1/2, 0$

(3) $x, y, z \cdot [u, v, w]$

(15) $4 \cdot -1/2, -1/2, z$

(4) $z, x, y \cdot [v, u, w]$

(16) $4 \cdot 1/2, 1/2, z$

(4) $x, y, z \cdot [u, v, w]$  

Generators selected

(1); $t' (1,0,0)$; $t' (0,1,0)$; $t' (0,0,1)$; (2); (3); (5); (13); (25).

Positions  
Continued

<table>
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<tr>
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<th>Wyckoff letter, Multiplicity</th>
<th>Coordinates</th>
<th>Generators selected</th>
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<td>(1); $t' (1,0,0)$; $t' (0,1,0)$; $t' (0,0,1)$; (2); (3); (5); (13); (25).</td>
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</tr>
<tr>
<td>48</td>
<td>m</td>
<td>m'</td>
<td>x,x,z [u,w,u]</td>
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<td>m'</td>
<td>x,x,z [u,w,u]</td>
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<td>m'</td>
<td>x,x,z [u,u,w]</td>
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<td>m'</td>
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Continued
### Symmetry of Special Projections

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<tr>
<th>Number</th>
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<th>Symbol</th>
<th>Origin</th>
<th>Transformation</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>mm'2'.. x,1/2,0 [0,0,w]</td>
<td>x,1/2,0 [0,0,w]</td>
<td>0,x,1/2 [w,0,0]</td>
<td>0,x,1/2 [w,0,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,0,x [0,w,0]</td>
<td>1/2,0,x [0,w,0]</td>
<td>1/2,x,0 [0,0,w]</td>
<td>1/2,x,0 [0,0,w]</td>
</tr>
<tr>
<td></td>
<td>x,0,1/2 [0,w,0]</td>
<td>x,0,1/2 [0,w,0]</td>
<td>0,1/2,x [w,0,0]</td>
<td>0,1/2,x [w,0,0]</td>
</tr>
<tr>
<td>16</td>
<td>.3m' x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
<td>x,x,x [u,u,u]</td>
</tr>
<tr>
<td></td>
<td>12 f 4m'.m' x,1/2,1/2 [u,0,0]</td>
<td>x,1/2,1/2 [u,0,0]</td>
<td>1/2,x,1/2 [0,u,0]</td>
<td>1/2,x,1/2 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td>1/2,1/2,0 [u,0,0]</td>
<td>1/2,1/2,0 [u,0,0]</td>
<td>1/2,1/2,0 [u,0,0]</td>
<td>1/2,1/2,0 [u,0,0]</td>
</tr>
<tr>
<td>12</td>
<td>e 4'm.m' x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
</tr>
<tr>
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<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
<td>0,0,x [0,0,0]</td>
<td>0,0,x [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>d 4'/m'm.m' 1/2,0,0 [0,0,0]</td>
<td>0,1/2,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>6</td>
<td>c 4/mm'.m' 1/2,1/2,0 [u,0,0]</td>
<td>1/2,0,1/2 [0,u,0]</td>
<td>1/2,1/2,0 [0,u,0]</td>
<td>1/2,1/2,0 [0,u,0]</td>
</tr>
<tr>
<td>2</td>
<td>b m3m' 1/2,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>a m3m' 0,0,0 [0,0,0]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry Symbols

- **mm'2':** Along [0,0,1] p4mm1'
  - \( a^* = a, b^* = b \)
  - Origin at 0,0,0

- **.3m':** Along [1,1,1] p6mm1'
  - \( a^* = (2a - b - c)/3, b^* = (-a + 2b - c)/3 \)
  - Origin at x,x,x

- **m3m':** Along [1,1,0] p-2mm
  - \( a^* = (a + b)/2, b^* = c \)
  - Origin at x,x,1/2
**Origin** at 432, at -1/4,-1/4,-1/4 from center (3)

**Asymmetric unit**
- \(0 \leq x \leq 1/2;\)
- \(0 \leq y \leq 1/2;\)
- \(0 \leq z \leq 1/2;\)
- \(y \leq x;\)
- \(z \leq y\)

**Vertices**
- \((0,0,0)\)
- \((1/2,0,0)\)
- \((1/2,1/2,0)\)
- \((1/2,1/2,1/2)\)

**Symmetry Operations**

1. \(1\)
2. \(2 \ 0,0,z\)
3. \(2 \ 0,y,0\)
4. \(2 \ x,0,0\)
5. \(3^+ \ x,x,x\)
6. \(3^+ \ x,x,x\)
7. \(3^+ \ x,x,x\)
8. \(3^+ \ x,x,x\)
9. \(3^- \ x,x,x\)
10. \(3^- \ x,x,x\)
11. \(3^- \ x,x,x\)
12. \(3^- \ x,x,x\)
Continued 222.1.1601 Pn̄3n

| (13) 2 | x,x,0  | (14) 2 | x,x,0  | (15) 4 | 0,0,z  | (16) 4 | 0,0,z  |
| (2_{xyz}) | 0,0,0 | (2_{xyz}) | 0,0,0 | (4_{z}) | 0,0,0 | (4_{z}) | 0,0,0 |
| (17) 4 | x,0,0  | (18) 2 | 0,y,y  | (19) 2 | 0,y,y  | (20) 4 | x,0,0  |
| (4_{x}) | 0,0,0 | (2_{yz}) | 0,0,0 | (2_{yz}) | 0,0,0 | (4_{x}) | 0,0,0 |
| (21) 4 | 0,y,0  | (22) 2 | x,0,x  | (23) 4 | 0,y,0  | (24) 2 | x,0,x  |
| (4_{y}) | 0,0,0 | (2_{wx}) | 0,0,0 | (4_{y}) | 0,0,0 |
| (25) \bar{1} | 1/4,1/4,1/4 | (26) n | (1/2,1/2,0) | x,y,z | (27) n | (1/2,0,1/2) | x,1/4,z | (28) n | (1/2,1/2,1/2) |
| (1) | 1/2,1/2,1/2 | (m_{yz}) | 1/2,1/2,12 | (m_{yz}) | 1/2,1/2,12 | |
| (29) 3^{+} | x,x,x; | 1/4,1/4,1/4 | (30) 3^{+} | x,-1,x; | -1/4,1/4,3/4 | (31) 3^{+} | x,x+1,x; | 1/4,3/4,-1/4 | (32) 3^{+} | x+1,x,x; | 3/4,-1/4,1/4 |
| (3_{xyz}) | 1/2,1/2,12 | (3_{xyz}) | 1/2,1/2,12 | (3_{xyz}) | 1/2,1/2,12 | |
| (33) 3^{-} | x,x,x; | 1/4,1/4,1/4 | (34) 3^{-} | x+1,-x,-x; | 1/4,-1/4,3/4 | (35) 3^{-} | x,x+1,-x+1; | -1/4,3/4,-1/4 | (36) 3^{-} | x+1,-x,-x; | 3/4,1/4,1/4 |
| (3_{xyz}) | 1/2,1/2,12 | (3_{xyz}) | 1/2,1/2,12 | (3_{xyz}) | 1/2,1/2,12 | |
| (37) c | (0,0,1/2) | x+1/2,\bar{x},-z | (38) n | (1/2,1/2,1/2) | x,x,z | (39) 4^{-} | 0,1/2,z; | 0,1/2,1/4 | (40) 4^{+} | 1/2,0,z; | 1/2,0,1/4 |
| (m_{wy}) | 1/2,1/2,12 | (m_{wy}) | 1/2,1/2,12 | (4_{z}) | 1/2,1/2,12 | (4_{z}) | 1/2,1/2,12 | |
| (41) 4^{-} | x,0,1/2; | 1/4,0,1/2 | (42) a | (1/2,0,0) | x,y+1/2,y | (43) n | (1/2,1/2,1/2) | x,y,y | (44) 4^{+} | x,1/2,0; | 1/4,1/2,0 |
| (4_{x}) | 1/2,1/2,12 | (m_{wy}) | 1/2,1/2,12 | (4_{z}) | 1/2,1/2,12 | (4_{x}) | 1/2,1/2,12 | |
| (45) 4^{+} | 0,y,1/2; | 0,1/4,1/2 | (46) b | (0,1/2,0) | x+1/2,y,x | (47) 4^{-} | 1/2,y,0; | 1/2,1/4,0 | (4^{+}) | 1/2,1/2,12 |
| (4_{y}) | 1/2,1/2,12 | (m_{wy}) | 1/2,1/2,12 | (4_{y}) | 1/2,1/2,12 | |

**Generators selected** (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Site Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wyckoff letter</td>
<td>Coordinates</td>
</tr>
</tbody>
</table>

48 i 1

| (1) x,y,z [u,v,w] | (2) \bar{x}, \bar{y},z [\bar{u}, \bar{v}, \bar{w}] | (3) \bar{x},y,z [\bar{u},v,w] | (4) x,\bar{y},\bar{z} [u,\bar{v},\bar{w}] |
| (5) z,x,y [w,u,v] | (6) z,\bar{x},y [w,\bar{u},\bar{v}] | (7) \bar{z},x,y [\bar{w},u,v] | (8) \bar{z},x,\bar{y} [\bar{w},u,\bar{v}] |
| (9) y,z,x [v,w,u] | (10) \bar{y},z,\bar{x} [\bar{v},w,u] | (11) y,\bar{z},\bar{x} [v,\bar{w},u] | (12) \bar{y},z,\bar{x} [\bar{v},\bar{w},u] |
| (13) y,x,z [v,u,\bar{w}] | (14) \bar{y},x,\bar{z} [\bar{v},u,\bar{w}] | (15) y,\bar{z},\bar{x} [u,\bar{w},\bar{v}] | (16) \bar{y},x,\bar{z} [\bar{v},u,\bar{w}] |
| (17) x,z,y [u,w,\bar{v}] | (18) \bar{x},z,\bar{y} [\bar{u},w,\bar{v}] | (19) x,\bar{z},y [u,\bar{w},v] | (20) x,\bar{z},\bar{y} [u,\bar{w},\bar{v}] |
| (21) z,y,x [v,w,\bar{u}] | (22) \bar{z},\bar{y},x [\bar{v},w,\bar{u}] | (23) z,y,\bar{x} [w,\bar{v},u] | (24) \bar{z},y,\bar{x} [\bar{v},w,\bar{u}] |
| (25) \bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2 [u,v,w] | (26) x+1/2,y+1/2,z+1/2 [u,\bar{v},\bar{w}] | (27) x+1/2,\bar{y}+1/2,z+1/2 [\bar{u},v,\bar{w}] | (28) \bar{x}+1/2,y+1/2,z+1/2 [u,\bar{v},\bar{w}] |
| (29) \bar{z}+1/2,x+1/2,\bar{y}+1/2 [w,u,\bar{v}] | (30) \bar{z}+1/2,x+1/2,\bar{y}+1/2 [\bar{w},u,\bar{v}] | (31) z+1/2,x+1/2,\bar{y}+1/2 [w,u,\bar{v}] | (32) z+1/2,x+1/2,\bar{y}+1/2 [w,u,\bar{v}] |
| (33) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [v,w,u] | (34) y+1/2,\bar{z}+1/2,x+1/2 [v,\bar{w},u] | (35) y+1/2,\bar{z}+1/2,x+1/2 [v,\bar{w},u] | (36) y+1/2,\bar{z}+1/2,x+1/2 [v,\bar{w},u] |
### Symmetry of Special Projections

Along $[0,0,1]$ p4mm1$'$

- $a^* = \frac{(a - b)/2}{2}$
- $b^* = \frac{(a + b)/2}{2}$

Origin at $0,0,z$

Along $[1,1,1]$ p6'm'm

- $a^* = \frac{(2a - b - c)/3}{2}$
- $b^* = \frac{(-a + 2b - c)/3}{2}$

Origin at $x,x,x$

Along $[1,1,0]$ p2mm1$'$

- $a^* = \frac{(-a + b)/2}{2}$
- $b^* = \frac{c/2}{2}$

Origin at $x,x,0$
Pn3n1'   m3m1'   Cubic
222.2.1602   P4/n32/n1'

Origin at 4321', at -1/4,-1/4,-1/4 from center (3 1')

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/2; y ≤ x; z ≤ y

Vertices
0,0,0 1/2,0,0 1/2,1/2,0 1/2,1/2,1/2

Symmetry Operations

For 1 + set

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) 0,0,0

(3) 2 0,y,0
(3) 0,0,0

(4) 2 x,0,0
(4) 0,0,0

(5) 3+ x,x,x
(3xyz | 0,0,0)

(6) 3+ x,x,x
(3xyz-1 | 0,0,0)

(7) 3+ x,x,x
(3xyz-1 | 0,0,0)

(8) 3+ x,x,x
(3xyz-1 | 0,0,0)

(9) 3- x,x,x
(3xyz-1 | 0,0,0)

(10) 3- x,x,x
(3xyz | 0,0,0)

(11) 3- x,x,x
(3xyz | 0,0,0)

(12) 3- x,x,x
(3xyz | 0,0,0)
Continued 222.2.1602 Pn3n1'

(13) 2' x,x,0
(2,0,0,0)
(14) 2' x,x,0
(2,0,0,0)
(15) 4'-0,0,0
(4',0,0,0)
(16) 4'-0,0,0
(4',0,0,0)

(17) 4' x,0,0
(4',0,0,0)
(18) 2' 0,y,y
(2,0,0,0)
(19) 2' 0,y,y
(2,0,0,0)
(20) 4' x,0,0
(4,0,0,0)

(21) 4' 0,y,0
(4,0,0,0)
(22) 2 0,y,0
(2,0,0,0)
(23) 4' 0,y,0
(4',0,0,0)
(24) 2 0,y,0
(2,0,0,0)

(25) 1/4,1/4,1/4
(1/2,1/2,1/2)
(26) n (1/2,1/2,0) x,y,1/4
(m,1/2,1/2,1/2)
(27) n (1/2,0,1/2) x,1/4,z
(m,1/2,1/2,1/2)
(28) n (0,1/2,1/2) 1/4,y,z
(m,1/2,1/2,1/2)

(29) 3' x,x,x; 1/4,1/4,1/4
(3,1/2,1/2,1/2)
(30) 3' x,x,x; 1/4,1/4,3/4
(3,1/2,1/2,1/2)
(31) 3' x,x,x; 1/4,3/4,-1/4
(3,1/2,1/2,1/2)
(32) 3' x,x,x; 3/4,-1/4,1/4
(3,1/2,1/2,1/2)

(33) 3' x,x,x; 1/4,1/4,1/4
(3,1/2,1/2,1/2)
(34) 3' x,x,x; 1/4,1/4,3/4
(3,1/2,1/2,1/2)
(35) 3' x,x,x; -1/4,3/4,1/4
(3,1/2,1/2,1/2)
(36) 3' x,x,x; 3/4,1/4,-1/4
(3,1/2,1/2,1/2)

(37) c (0,0,1/2) x+1/2,x,z
(m,1/2,1/2,1/2)
(38) n (1/2,1/2,1/2) x,x,z
(m,1/2,1/2,1/2)
(39) 4' 0,1/2,z; 0,1/2,1/4
(4',1/2,1/2,1/2)
(40) 4' 1/2,0,z; 1/2,0,1/4
(4',1/2,1/2,1/2)

(41) 4' x,0,1/2; 1/4,0,1/2
(4',1/2,1/2,1/2)
(42) a (1/2,0,0) x,y+1/2,y
(m,1/2,1/2,1/2)
(43) n (1/2,1/2,1/2) x,y,y
(m,1/2,1/2,1/2)
(44) 4' x,1/2,0; 1/4,1/2,0
(4',1/2,1/2,1/2)

(45) 4' 0,y,1/2; 0,1/4,1/2
(4,1/2,1/2,1/2)
(46) b (0,1/2,0) x+1/2,y,x
(m,1/2,1/2,1/2)
(47) 4' 1/2,y,0; 1/2,1/4,0
(4',1/2,1/2,1/2)
(48) n (1/2,1/2,1/2) x,y,x
(m,1/2,1/2,1/2)

For 1' + set

(1) 1'
(0,0,0)
(2) 2' 0,0,z
(2,0,0,0)
(3) 2' 0,y,0
(2',0,0,0)
(4) 2' x,0,0
(2',0,0,0)

(5) 3' x,x,x
(3,0,0,0)
(6) 3' x,x,x
(3,0,0,0)
(7) 3' x,x,x
(3,0,0,0)
(8) 3' x,x,x
(3,0,0,0)

(9) 3' x,x,x
(3,0,0,0)
(10) 3' x,x,x
(3,0,0,0)
(11) 3' x,x,x
(3,0,0,0)
(12) 3' x,x,x
(3,0,0,0)

(13) 2' x,x,0
(2,0,0,0)
(14) 2' x,x,0
(2,0,0,0)
(15) 4' 0,0,0
(4',0,0,0)
(16) 4' 0,0,0
(4',0,0,0)

(17) 4' 0,y,0
(4',0,0,0)
(18) 2' 0,y,0
(2,0,0,0)
(19) 2' 0,y,0
(2',0,0,0)
(20) 4' 0,y,0
(4,0,0,0)

(21) 4' 0,y,0
(4,0,0,0)
(22) 2' x,0,x
(2,0,0,0)
(23) 4' 0,y,0
(4',0,0,0)
(24) 2' x,0,x
(2,0,0,0)

(25) 1' 1/4,1/4,1/4
(1/2,1/2,1/2)
(26) n' (1/2,1/2,0) x,y,1/4
(m',1/2,1/2,1/2)
(27) n' (1/2,0,1/2) x,1/4,z
(m',1/2,1/2,1/2)
(28) n' (0,1/2,1/2) 1/4,y,z
(m',1/2,1/2,1/2)

(29) 3' x,x,x; 1/4,1/4,1/4
(3,1/2,1/2,1/2)
(30) 3' x,x,x; 1/4,1/4,3/4
(3,1/2,1/2,1/2)
(31) 3' x,x,x; 1/4,3/4,-1/4
(3,1/2,1/2,1/2)
(32) 3' x,x,x; 3/4,-1/4,1/4
(3,1/2,1/2,1/2)

(33) 3' x,x,x; 1/4,1/4,1/4
(3,1/2,1/2,1/2)
(34) 3' x,x,x; 1/4,1/4,3/4
(3,1/2,1/2,1/2)
(35) 3' x,x,x; -1/4,3/4,1/4
(3,1/2,1/2,1/2)
(36) 3' x,x,x; 3/4,1/4,-1/4
(3,1/2,1/2,1/2)
Continued

| (37) c' (0,0,1/2) x+1/2,\bar{x},z | (38) n' (1/2,1/2,1/2) x,x,z | (39) \bar{4} \cdot \bar{1} 0,1/2,z; 0,1/2,1/4 | (40) \bar{4} \cdot \bar{1} 1/2,0,z; 1/2,0,1/4 |
| \begin{align*} (m_{xy} & | 1/2,1/2,12) \end{align*} | \begin{align*} (m_{xy} & | 1/2,1/2,12) \end{align*} | \begin{align*} (m_{yz} & | 1/2,1/2,12) \end{align*} | \begin{align*} (m_{yz} & | 1/2,1/2,12) \end{align*} |

| (41) \bar{4} \cdot \bar{1} x,0,1/2; 1/4,0,1/2 | (42) a' (1/2,2,0,0) x,y+1/2,\bar{y} | (43) n' (1/2,1/2,1/2) x,y,y | (44) \bar{4} \cdot \bar{1} x,1/2,0; 1/4,1/2,0 |
| \begin{align*} (4 \bar{m} x & \bar{y} \bar{z} | 1/2,1/2,12) \end{align*} | \begin{align*} (4 \bar{m} x & \bar{z} | 1/2,1/2,12) \end{align*} | \begin{align*} (4 \bar{m} x & \bar{z} | 1/2,1/2,12) \end{align*} | \begin{align*} (4 \bar{m} x & \bar{z} | 1/2,1/2,12) \end{align*} |

| (45) \bar{4} \cdot \bar{1} 0,y,1/2; 1/4,1/2 | (46) b' (0,1/2,0) x+1/2,y,\bar{x} | (47) \bar{4} \cdot \bar{1} 1/2,y,0; 1/2,1/4,0 | (48) \bar{n} (1/2,1/2,1/2) x,y,x |
| \begin{align*} (4 \bar{m} y & \bar{z} \bar{x} | 1/2,1/2,12) \end{align*} | \begin{align*} (4 \bar{m} y & \bar{z} \bar{x} | 1/2,1/2,12) \end{align*} | \begin{align*} (4 \bar{m} x & \bar{z} \bar{y} | 1/2,1/2,12) \end{align*} | \begin{align*} (4 \bar{m} x & \bar{z} \bar{y} | 1/2,1/2,12) \end{align*} |

Generators selected

1; t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25); 1'.

Positions

| Multiplicity, Wyckoff letter, Site Symmetry. |
| Coordinates |
| 1 + | 1' + |

| (1) x,y,z [0,0,0] | (2) x,y,z [0,0,0] | (3) x,y,z [0,0,0] | (4) x,y,z [0,0,0] |
| (5) z,x,y [0,0,0] | (6) z,x,y [0,0,0] | (7) z,x,y [0,0,0] | (8) z,x,y [0,0,0] |
| (9) y,z,x [0,0,0] | (10) y,z,x [0,0,0] | (11) y,z,x [0,0,0] | (12) y,z,x [0,0,0] |
| (13) y,z,x [0,0,0] | (14) y,z,x [0,0,0] | (15) y,z,x [0,0,0] | (16) y,z,x [0,0,0] |
| (17) x,z,y [0,0,0] | (18) x,z,y [0,0,0] | (19) x,z,y [0,0,0] | (20) x,z,y [0,0,0] |
| (21) z,y,x [0,0,0] | (22) z,y,x [0,0,0] | (23) z,y,x [0,0,0] | (24) z,y,x [0,0,0] |
| (25) \bar{x}+1/2,\bar{y}+1/2,\bar{z}+1/2 [0,0,0] | (26) x+1/2,y+1/2,z+1/2 [0,0,0] | (27) x+1/2,y+1/2,z+1/2 [0,0,0] | (28) \bar{x}+1/2,y+1/2,z+1/2 [0,0,0] |
| (29) \bar{z}+1/2,\bar{x}+1/2,\bar{y}+1/2 [0,0,0] | (30) \bar{z}+1/2,\bar{x}+1/2,\bar{y}+1/2 [0,0,0] | (31) \bar{z}+1/2,\bar{x}+1/2,\bar{y}+1/2 [0,0,0] | (32) \bar{z}+1/2,\bar{x}+1/2,\bar{y}+1/2 [0,0,0] |
| (33) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] | (34) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] | (35) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] | (36) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] |
| (37) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] | (38) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] | (39) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] | (40) \bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [0,0,0] |
| (41) \bar{x}+1/2,\bar{z}+1/2,\bar{y}+1/2 [0,0,0] | (42) \bar{x}+1/2,\bar{z}+1/2,\bar{y}+1/2 [0,0,0] | (43) \bar{x}+1/2,\bar{z}+1/2,\bar{y}+1/2 [0,0,0] | (44) \bar{x}+1/2,\bar{z}+1/2,\bar{y}+1/2 [0,0,0] |
| (45) \bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [0,0,0] | (46) \bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [0,0,0] | (47) \bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [0,0,0] | (48) \bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [0,0,0] |
| 24 h \quad ..21' |

<p>| 0,y,z [0,0,0] | 0,y,z [0,0,0] | 0,y,z [0,0,0] | 0,y,z [0,0,0] |
| y,0,z [0,0,0] | y,0,z [0,0,0] | y,0,z [0,0,0] | y,0,z [0,0,0] |
| y,y,z [0,0,0] | y,y,z [0,0,0] | y,y,z [0,0,0] | y,y,z [0,0,0] |</p>
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<td>1/2, $\tilde{y} + 1/2, y + 1/2$ [0,0,0]</td>
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<tr>
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<td>$y + 1/2, 1/2, y + 1/2$ [0,0,0]</td>
<td>$y + 1/2, 1/2, \bar{y} + 1/2$ [0,0,0]</td>
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<tr>
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<td>$y + 1/2, \bar{y} + 1/2, 1/2$ [0,0,0]</td>
<td>$y + 1/2, y + 1/2, 1/2$ [0,0,0]</td>
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<td>x,0,1/2 [0,0,0]</td>
<td>$x,0,1/2$ [0,0,0]</td>
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<tr>
<td>16 f 3..1'</td>
<td>x,x,x [0,0,0]</td>
<td>$x,x,x$ [0,0,0]</td>
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<tr>
<td>12 e 4..1'</td>
<td>x,0,0 [0,0,0]</td>
<td>$x,0,0$ [0,0,0]</td>
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<tr>
<td>12 d 4'..1'</td>
<td>1/4,0,1/2 [0,0,0]</td>
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<td>8 c 3'..1'</td>
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<td>6 b 42.21'</td>
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Symmetry of Special Projections

Along $[0,0,1]$ p4mm$1'$

\[
a^* = \frac{a - b}{2} \quad b^* = \frac{a + b}{2}
\]
-origin at $0,0,z$

Along $[1,1,1]$ p6mm$1'$

\[
a^* = \frac{2a - b - c}{3} \quad b^* = \frac{-a + 2b - c}{3}
\]
-origin at $x,x,x$

Along $[1,1,0]$ p2mm$1'$

\[
a^* = \frac{-a + b}{2} \quad b^* = \frac{c}{2}
\]
-origin at $x,x,0$
Origin at 4'32', at -1/4,-1/4,-1/4 from center (3')

Asymmetric unit

Vertices

Symmetry Operations

(1) 1
(1) 0,0,0

(2) 2 0,0,z
(2) 0,0,0

(3) 2 0,y,0
(3) 0,0,0

(4) 2 x,0,0
(4) 0,0,0

(5) 3' x,x,x
(3) x,y,z

(6) 3' x,x,x
(6) x,y,z

(7) 3' x,x,x
(7) x,y,z

(8) 3' x,x,x
(8) x,y,z

(9) 3' x,x,x
(3) x,y,z

(10) 3' x,x,x
(3) x,y,z

(11) 3' x,x,x
(3) x,y,z

(12) 3' x,x,x
(3) x,y,z
Continued

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<th>(3) x,y,z [u,v,w]</th>
<th>(4) x,y,z [u,v,w]</th>
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<td>(5) z,x,y [w,u,v]</td>
<td>(6) z,x,y [w,u,v]</td>
<td>(7) z,x,y [w,u,v]</td>
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<tr>
<td>3</td>
<td>y,z,x [v,w,u]</td>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) y,z,x [v,w,u]</td>
<td>(11) y,z,x [v,w,u]</td>
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<td>4</td>
<td>y,z,x [v,w,u]</td>
<td>(13) y,z,x [v,w,u]</td>
<td>(14) y,z,x [v,w,u]</td>
<td>(15) y,z,x [v,w,u]</td>
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<td>x,y,z [u,v,w]</td>
<td>(29) x,y,z [u,v,w]</td>
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<td>9</td>
<td>x,y,z [u,v,w]</td>
<td>(33) x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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<td>x,y,z [u,v,w]</td>
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<td>(51) x,y,z [u,v,w]</td>
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<td>(54) x,y,z [u,v,w]</td>
<td>(55) x,y,z [u,v,w]</td>
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<td>(58) x,y,z [u,v,w]</td>
<td>(59) x,y,z [u,v,w]</td>
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### Symmetry of Special Projections

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<td>a</td>
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<td>$0,0,0 [0,0,0]$</td>
<td>$1/2,1/2,1/2 [0,0,0]$</td>
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#### Representations

**Along $[0,0,1]$**
- $p4m'm'$
  - $a^* = (a - b)/2$
  - $b^* = (a + b)/2$
  - Origin at $0,0,z$

**Along $[1,1,1]$**
- $p6mm$
  - $a^* = (2a - b - c)/3$
  - $b^* = (-a + 2b - c)/3$
  - Origin at $x,x,x$

**Along $[1,1,0]$**
- $p2m'm'$
  - $a^* = (-a + b)/2$
  - $b^* = c/2$
  - Origin at $x,x,1/4$
Origin at 4'32, at -1/4,-1/4,-1/4 from center (3)

Asymmetric unit

\(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/2; \quad y \leq x; \quad z \leq y\)

Vertices

\(0,0,0, \quad 1/2,0,0, \quad 1/2,1/2,0, \quad 1/2,1/2,1/2\)

Symmetry Operations

\begin{align*}
(1) \ 1 & \quad (2) \ 2 \ 0,0,z \quad (3) \ 2 \ 0,y,0 \quad (4) \ 2 \ x,0,0 \\
(1\mid0,0,0) & \quad (2\mid0,0,0) \quad (2\mid0,0,0) \quad (2\mid0,0,0) \\
(5) \ 3^+ \ x,x,x & \quad (6) \ 3^+ \ x,x,x \quad (7) \ 3^+ \ x,x,x \quad (8) \ 3^+ \ x,x,x \\
(3_{xyz}\mid0,0,0) & \quad (3_{xyz}\mid0,0,0) \quad (3_{xyz}\mid0,0,0) \quad (3_{xyz}\mid0,0,0) \\
(9) \ 3^- \ x,x,x & \quad (10) \ 3^- \ x,x,x \quad (11) \ 3^- \ x,x,x \quad (12) \ 3^- \ x,x,x \\
(3_{xyz}^{-1}\mid0,0,0) & \quad (3_{xyz}^{-1}\mid0,0,0) \quad (3_{xyz}^{-1}\mid0,0,0) \quad (3_{xyz}^{-1}\mid0,0,0)
\end{align*}
Continued

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

48 i 1

(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w]
(5) z,x,y [w,u,v] (6) z,x,y [w,u,v] (7) z,x,y [w,u,v] (8) z,x,y [w,u,v]
(9) y,z,x [v,w,u] (10) y,z,x [v,w,u] (11) y,z,x [v,w,u] (12) y,z,x [v,w,u]
(13) x,y,z [u,v,w] (14) x,y,z [u,v,w] (15) x,y,z [u,v,w] (16) x,y,z [u,v,w]
(17) x,y,z [u,v,w] (18) x,y,z [u,v,w] (19) x,y,z [u,v,w] (20) x,y,z [u,v,w]
(21) x,y,z [u,v,w] (22) x,y,z [u,v,w] (23) x,y,z [u,v,w] (24) x,y,z [u,v,w]

(25) x+1/2, y+1/2, z+1/2 [u,v,w] (26) x+1/2, y+1/2, z+1/2 [u,v,w] (27) x+1/2, y+1/2, z+1/2 [u,v,w] (28) x+1/2, y+1/2, z+1/2 [u,v,w]
(29) z+1/2, x+1/2, y+1/2 [w,u,v] (30) z+1/2, x+1/2, y+1/2 [w,u,v] (31) z+1/2, x+1/2, y+1/2 [w,u,v] (32) z+1/2, x+1/2, y+1/2 [w,u,v]
(33) y+1/2, z+1/2, x+1/2 [v,w,u] (34) y+1/2, z+1/2, x+1/2 [v,w,u] (35) y+1/2, z+1/2, x+1/2 [v,w,u] (36) y+1/2, z+1/2, x+1/2 [v,w,u]
<table>
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<tr>
<th>12</th>
<th>d</th>
<th>4'..</th>
<th>1/4,0,1/2 [0,0,0]</th>
<th>3/4,0,1/2 [0,0,0]</th>
<th>1/2,1/4 [0,0,0]</th>
<th>1/2,3/4,0 [0,0,0]</th>
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<td>1/2,0,3/4 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
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<td>6</td>
<td>b</td>
<td>4'2.2'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<td>1/2,0,0 [0,0,0]</td>
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<td>0,0,1/2 [0,0,0]</td>
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<tr>
<td>2</td>
<td>a</td>
<td>4'32'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
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</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
\( \mathbf{a}^* = \frac{(\mathbf{a} - \mathbf{b})}{2} \quad \mathbf{b}^* = \frac{(\mathbf{a} + \mathbf{b})}{2} \)  
Origin at 0,0,z

Along [1,1,1] p6'mm'  
\( \mathbf{a}^* = \frac{(2\mathbf{a} - \mathbf{b} - \mathbf{c})}{3} \quad \mathbf{b}^* = \frac{(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})}{3} \)  
Origin at x,x,x

Along [1,1,0] p2'mm'  
\( \mathbf{a}^* = \frac{\mathbf{c}}{2} \quad \mathbf{b}^* = \frac{(-\mathbf{a} + \mathbf{b})}{2} \)  
Origin at x,x,0
Origin at 432, at -1/4,-1/4,-1/4 from center ($3^*$)

Asymmetric unit: 
- $0 \leq x \leq 1/2$
- $0 \leq y \leq 1/2$
- $0 \leq z \leq 1/2$
- $y \leq x$
- $z \leq y$

Vertices: 
- $0,0,0$
- $1/2,0,0$
- $1/2,1/2,0$
- $1/2,1/2,1/2$

Symmetry Operations:

1. $1$
   - $(1|0,0,0)$

2. $2$ 0,0,z
   - $(2|_2|0,0,0)$

3. $2$ 0,y,0
   - $(2|_{y}|0,0,0)$

4. $2$ x,0,0
   - $(2|x|0,0,0)$

5. $3^*$ x,x,x
   - $(3_{xyz}|0,0,0)$

6. $3^*$ x,x,x
   - $(3_{xyz}|0,0,0)$

7. $3^*$ x,x,x
   - $(3_{xyz}|0,0,0)$

8. $3^*$ x,x,x
   - $(3_{xyz}|0,0,0)$

9. $3^*$ x,x,x
   - $(3_{xyz}|0,0,0)$

10. $3^*$ x,x,x
    - $(3_{xyz}|0,0,0)$

11. $3^*$ x,x,x
    - $(3_{xyz}|0,0,0)$

12. $3^*$ x,x,x
    - $(3_{xyz}|0,0,0)$

222.5.1605 - 1 - 3667
Continued 222.5.1605 Pn'3'n'

Generators selected (1): t(1,0,0); t(0,1,0); t(0,0,1); (2): (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48 i 1

(1) x,y,z [u,v,w] (2) x,y,z [u,v,w] (3) x,y,z [u,v,w] (4) x,y,z [u,v,w] (5) z,x,y [w,u,v] (6) z,x,y [w,u,v] (7) z,x,y [w,u,v] (8) z,x,y [w,u,v] (9) y,z,x [v,w,u] (10) y,z,x [v,w,u] (11) y,z,x [v,w,u] (12) y,z,x [v,w,u] (13) x,z,y [u,v,w] (14) x,z,y [u,v,w] (15) x,z,y [u,v,w] (16) x,z,y [u,v,w] (17) z,y,x [w,u,v] (18) z,y,x [w,u,v] (19) z,y,x [w,u,v] (20) z,y,x [w,u,v] (21) z,y,x [w,u,v] (22) z,y,x [w,u,v] (23) z,y,x [w,u,v] (24) z,y,x [w,u,v] (25) x+1/2,y+1/2,z+1/2 [u,v,w] (26) x+1/2,y+1/2,z+1/2 [u,v,w] (27) x+1/2,y+1/2,z+1/2 [u,v,w] (28) x+1/2,y+1/2,z+1/2 [u,v,w] (29) z+1/2,x+1/2,y+1/2 [w,u,v] (30) z+1/2,x+1/2,y+1/2 [w,u,v] (31) z+1/2,x+1/2,y+1/2 [w,u,v] (32) z+1/2,x+1/2,y+1/2 [w,u,v] (33) y+1/2,z+1/2,x+1/2 [v,w,u] (34) y+1/2,z+1/2,x+1/2 [v,w,u] (35) y+1/2,z+1/2,x+1/2 [v,w,u] (36) y+1/2,z+1/2,x+1/2 [v,w,u]
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<td>222.5.1605 Pn′3’n’</td>
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<td>x+1/2, x+1/2, x+1/2 [u,u,u] x+1/2, x+1/2, x+1/2 [u,u,u] x+1/2, x+1/2, x+1/2 [u,u,u]</td>
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<td>x,0,0 [u,0,0] x,0,0 [u,0,0] x,0,0 [u,0,0] 0,x,0 [0,u,0]</td>
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<td>x+1/2,1/2,1/2 [u,0,0] x+1/2,1/2,1/2 [u,0,0] 1/2,x+1/2,1/2 [0,u,0] 1/2,x+1/2,1/2 [0,u,0]</td>
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<td>$\bar{3}'$..</td>
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<td>2</td>
<td>a</td>
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**Symmetry of Special Projections**

- **Along [0,0,1]**: p4m'm'
  - $a^* = (a - b)/2$
  - $b^* = (a + b)/2$
  - Origin at 0,0,z

- **Along [1,1,1]**: p6m'm'
  - $a^* = (2a - b - c)/3$
  - $b^* = (-a + 2b - c)/3$
  - Origin at x,x,x

- **Along [1,1,0]**: p2m'm'
  - $a^* = (-a + b)/2$
  - $b^* = c/2$
  - Origin at x,x,0
Origin at center ($m\bar{3}$)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad z \leq \min(x, 1/2-x, y, 1/2-y) \]

Vertices

| 0,0,0 | 1/2,0,0 | 1/2,1/2,0 | 0,1/2,0 | 1/4,1/4,1/4 |

Symmetry Operations

(1) 1  
(1) [0,0,0]  

(2) 2 0,0,z  
(2) [0,0,0]  

(3) 2 0,y,0  
(3) [0,0,0]  

(4) 2 x,0,0  
(4) [0,0,0]  

(5) 3^+ x,x,x  
(5) [xyz,0,0,0]  

(6) 3^+ x,x,x  
(6) [xyz,0,0,0]  

(7) 3^+ x,x,x  
(7) [xyz,0,0,0]  

(8) 3^+ x,x,x  
(8) [xyz,0,0,0]  

(9) 3^- x,x,x  
(9) [xyz^{-1},0,0,0]  

(10) 3^- x,x,x  
(10) [xyz^{-1},0,0,0]  

(11) 3^- x,x,x  
(11) [xyz^{-1},0,0,0]  

(12) 3^- x,x,x  
(12) [xyz^{-1},0,0,0]  

223.1.1606 - 1 - 3671
Continued 223.1.1606 Pm3n

(13) 2 (1/2, 1/2, 0) x, x, 1/4
(2x, y, z [u, v, w])

(14) 2 x, x+1/2, 1/4
(2x, y, z [u, v, w])

(15) 4 (0, 0, 1/2) 1/2, 0, z
(4x, y, z [u, v, w])

(16) 4+ (0, 0, 1/2) 0, 1/2, z
(4x, y, z [u, v, w])

(17) 4 (1/2, 0, 0) x, 1/2, 0
(4x, y, z [u, v, w])

(18) 2 (0, 1/2, 1/2) 1/4, y, y
(2x, y, z [u, v, w])

(19) 2 1/4, y+1/2, y
(2x, y, z [u, v, w])

(20) 4+ (1/2, 0, 0) x, 0, 1/2
(4x, y, z [u, v, w])

(21) 4* (0, 1/2, 0) 1/2, y, 0
(4x, y, z [u, v, w])

(22) 2 (1/2, 0, 1/2) x, 1/4, x
(2x, y, z [u, v, w])

(23) 4* (0, 1/2, 0) 0, y, 1/2
(4x, y, z [u, v, w])

(24) 2 y+1/2, 1/4, x
(2x, y, z [u, v, w])

(25) x, y, z [u, v, w]
(3x, y, z [u, v, w])

(26) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(27) m x, y, 0
(3x, y, z [u, v, w])

(28) m x, 0, z
(3x, y, z [u, v, w])

(29) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(30) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(31) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(32) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(33) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(34) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(35) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(36) 3+ x, x, x; 0, 0, 0
(3x, y, z [u, v, w])

(37) c (0, 0, 1/2) x+1/2, x, z
(m x, y, z [u, v, w])

(38) n (1/2, 1/2, 1/2) x, x, z
(m x, y, z [u, v, w])

(39) 4* 0, 1/2, z; 0, 1/2, 1/4
(4x, y, z [u, v, w])

(40) 4* 1/2, 0, z; 1/2, 0, 1/4
(4x, y, z [u, v, w])

(41) 4* x, 0, 1/2; 1/4, 0, 1/2
(4x, y, z [u, v, w])

(42) a (1/2, 0, 0) x, y+1/2, y
(m x, y, z [u, v, w])

(43) n (1/2, 1/2, 1/2) x, y, y
(m x, y, z [u, v, w])

(44) 4* x, 1/2, 0; 1/4, 1/2, 0
(4x, y, z [u, v, w])

(45) 4+ 0, y, 1/2; 0, 1/4, 1/2
(4x, y, z [u, v, w])

(46) b (0, 1/2, 0) x+1/2, y, x
(m x, y, z [u, v, w])

(47) 4* 1/2, y, 0; 1/2, 1/4, 0
(4x, y, z [u, v, w])

(48) n (1/2, 1/2, 1/2) x, y, x
(m x, y, z [u, v, w])

Generators selected (1): t(1, 0, 0); t(0, 1, 0); t(0, 0, 1); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48 1 1

(1) x, y, z [u, v, w]
(2) x, y, z [u, v, w]
(3) x, y, z [u, v, w]
(4) x, y, z [u, v, w]

(5) z, x, y [w, u, v]
(6) z, x, y [w, u, v]
(7) z, x, y [w, u, v]
(8) z, x, y [w, u, v]

(9) y, z, x [v, w, u]
(10) y, z, x [v, w, u]
(11) y, z, x [v, w, u]
(12) y, z, x [v, w, u]

(13) y+1/2, x+1/2, z+1/2 [v, w, u]
(14) y+1/2, x+1/2, z+1/2 [v, w, u]
(15) y+1/2, x+1/2, z+1/2 [v, w, u]
(16) y+1/2, x+1/2, z+1/2 [v, w, u]

(17) x+1/2, z+1/2, y+1/2 [w, v, u]
(18) x+1/2, z+1/2, y+1/2 [w, v, u]
(19) x+1/2, z+1/2, y+1/2 [w, v, u]
(20) x+1/2, z+1/2, y+1/2 [w, v, u]

(21) z+1/2, y+1/2, x+1/2 [w, v, u]
(22) z+1/2, y+1/2, x+1/2 [w, v, u]
(23) z+1/2, y+1/2, x+1/2 [w, v, u]
(24) z+1/2, y+1/2, x+1/2 [w, v, u]

(25) x, y, z [u, v, w]
(26) x, y, z [u, v, w]
(27) x, y, z [u, v, w]
(28) x, y, z [u, v, w]

(29) z, x, y [w, u, v]
(30) z, x, y [w, u, v]
(31) z, x, y [w, u, v]
(32) z, x, y [w, u, v]

(33) y, z, x [v, w, u]
(34) y, z, x [v, w, u]
(35) y, z, x [v, w, u]
(36) y, z, x [v, w, u]
Continued

(37) $y + 1/2, x + 1/2, z + 1/2 \ [v, u, w]$

(38) $y + 1/2, x + 1/2, z + 1/2 \ [v, u, w]$

(39) $y + 1/2, x + 1/2, z + 1/2 \ [v, u, w]$

(40) $y + 1/2, x + 1/2, z + 1/2 \ [v, u, w]$

(41) $x + 1/2, z + 1/2, y + 1/2 \ [u, w, v]$

(42) $x + 1/2, z + 1/2, y + 1/2 \ [u, w, v]$

(43) $x + 1/2, z + 1/2, y + 1/2 \ [u, w, v]$

(44) $x + 1/2, z + 1/2, y + 1/2 \ [u, w, v]$

(45) $z + 1/2, y + 1/2, x + 1/2 \ [w, v, u]$

(46) $z + 1/2, y + 1/2, x + 1/2 \ [w, v, u]$

(47) $z + 1/2, y + 1/2, x + 1/2 \ [w, v, u]$

(48) $z + 1/2, y + 1/2, x + 1/2 \ [w, v, u]$

24 $k \ m_. \ 0, y, z \ [u, 0, 0] \ 0, y, z \ [u, 0, 0] \ 0, y, z \ [u, 0, 0]$

$z, 0, y \ [0, u, 0] \ z, 0, y \ [0, u, 0] \ z, 0, y \ [0, u, 0]$

$y, z, 0 \ [0, 0, u] \ y, z, 0 \ [0, 0, u] \ y, z, 0 \ [0, 0, u]$

$y + 1/2, 1/2, z + 1/2 \ [0, u, 0] \ y + 1/2, 1/2, z + 1/2 \ [0, u, 0] y + 1/2, 1/2, z + 1/2 \ [0, u, 0]$

$1/2, z + 1/2, y + 1/2 \ [u, 0, 0] \ 1/2, z + 1/2, y + 1/2 \ [u, 0, 0] 1/2, z + 1/2, y + 1/2 \ [u, 0, 0]$

$z + 1/2, y + 1/2, 1/2 \ [0, 0, u] \ 1/2, z + 1/2, y + 1/2 \ [0, 0, u] \ 1/2, z + 1/2, y + 1/2 \ [0, 0, u]$

24 $j \ .2$

$1/4, y, y + 1/2 \ [0, v, v] \ 3/4, y, y + 1/2 \ [0, v, v] \ 3/4, y, y + 1/2 \ [0, v, v]$

$y + 1/2, 1/4, y \ [v, 0, v] \ y + 1/2, 1/4, y \ [v, 0, v] \ y + 1/2, 1/4, y \ [v, 0, v]$

$y, y + 1/2, 1/4 \ [v, v, 0] \ y, y + 1/2, 1/4 \ [v, v, 0] \ y, y + 1/2, 1/4 \ [v, v, 0]$

$3/4, y, y + 1/2 \ [0, v, v] \ 1/4, y, y + 1/2 \ [0, v, v] \ 1/4, y, y + 1/2 \ [0, v, v]$

$y + 1/2, 3/4, y \ [v, 0, v] \ y + 1/2, 3/4, y \ [v, 0, v] \ y + 1/2, 3/4, y \ [v, 0, v]$

$y, y + 1/2, 3/4 \ [v, v, 0] \ y, y + 1/2, 3/4 \ [v, v, 0] \ y, y + 1/2, 3/4 \ [v, v, 0]$

16 $i \ .3.$

$x, x, x \ [u, u, u] \ x, x, x \ [u, u, u] \ x, x, x \ [u, u, u]$

$x + 1/2, x + 1/2, x + 1/2 \ [u, u, u] \ x + 1/2, x + 1/2, x + 1/2 \ [u, u, u] \ x + 1/2, x + 1/2, x + 1/2 \ [u, u, u]$

$x, x, x \ [u, u, u] \ x, x, x \ [u, u, u] \ x, x, x \ [u, u, u]$

$x + 1/2, x + 1/2, x + 1/2 \ [u, u, u] \ x + 1/2, x + 1/2, x + 1/2 \ [u, u, u] \ x + 1/2, x + 1/2, x + 1/2 \ [u, u, u]$

12 $h \ mm2.$

$x, 1/2, 0 \ [0, 0, 0] \ x, 1/2, 0 \ [0, 0, 0] \ 0, x, 1/2 \ [0, 0, 0] \ 0, x, 1/2 \ [0, 0, 0]$

$1/2, 0, x \ [0, 0, 0] \ 1/2, 0, x \ [0, 0, 0] \ 0, x + 1/2, 1/2 \ [0, 0, 0] \ 0, x + 1/2, 1/2 \ [0, 0, 0]$

$x + 1/2, 1/2, 0 \ [0, 0, 0] \ x + 1/2, 1/2, 0 \ [0, 0, 0] \ 1/2, 0, x + 1/2 \ [0, 0, 0] \ 1/2, 0, x + 1/2 \ [0, 0, 0]$
Continued

| 12 g | mm2.. | \(x,0,1/2[0,0,0]\) | \(\overline{x},0,1/2[0,0,0]\) | \(1/2,x,0[0,0,0]\) | \(1/2,\overline{x},0[0,0,0]\) |
| 0,1/2,x | [0,0,0] | 0,1/2,\overline{x}[0,0,0] | \(1/2,\overline{x}+1/2,0[0,0,0]\) | \(1/2,\overline{x}+1/2,0[0,0,0]\) |
| \(x+1/2,0,1/2[0,0,0]\) | \(\overline{x}+1/2,0,1/2[0,0,0]\) | \(0,1/2,\overline{x}+1/2[0,0,0]\) | \(0,1/2,\overline{x}+1/2[0,0,0]\) |

| 12 f | mm2.. | \(x,0,0[0,0,0]\) | \(\overline{x},0,0[0,0,0]\) | \(0,x,0[0,0,0]\) | \(0,\overline{x},0[0,0,0]\) |
| 0,0,x | [0,0,0] | 0,0,\overline{x}[0,0,0] | \(1/2,x+1/2,1/2[0,0,0]\) | \(1/2,x+1/2,1/2[0,0,0]\) |
| \(x+1/2,1/2,1/2[0,0,0]\) | \(\overline{x}+1/2,1/2,1/2[0,0,0]\) | \(1/2,1/2,x+1/2[0,0,0]\) | \(1/2,1/2,x+1/2[0,0,0]\) |

| 8 e | .32 | \(1/4,1/4,1/4[0,0,0]\) | \(3/4,3/4,1/4[0,0,0]\) | \(3/4,1/4,3/4[0,0,0]\) | \(1/4,3/4,3/4[0,0,0]\) |
| \(3/4,3/4,3/4[0,0,0]\) | \(1/4,1/4,3/4[0,0,0]\) | \(1/4,3/4,1/4[0,0,0]\) | \(3/4,1/4,1/4[0,0,0]\) |

| 6 d | \(\overline{4}m.2\) | \(1/4,1/2,0[0,0,0]\) | \(3/4,1/2,0[0,0,0]\) | \(0,1/4,1/2[0,0,0]\) |
| 0,3/4,1/2 | [0,0,0] | 1/2,0,1/4[0,0,0] | \(1/2,0,3/4[0,0,0]\) |

| 6 c | \(\overline{4}m.2\) | \(1/4,0,1/2[0,0,0]\) | \(3/4,0,1/2[0,0,0]\) | \(1/2,1,4,0[0,0,0]\) |
| 1/2,3/4,0 | [0,0,0] | 0,1/2,1/4[0,0,0] | \(0,1/2,3/4[0,0,0]\) |

| 6 b | mmm.. | \(0,1/2,1/2[0,0,0]\) | \(1/2,0,1/2[0,0,0]\) | \(1/2,1,2,0[0,0,0]\) |
| 0,1/2,0 | [0,0,0] | 1/2,0,0[0,0,0] | \(0,0,1/2[0,0,0]\) |

| 2 a | m\(\overline{3}\). | \(0,0,0[0,0,0]\) | \(1/2,1/2,1/2[0,0,0]\) |

Symmetry of Special Projections

| Along \([0,0,1]\) | p4mm1' | \(a^* = a\) \(b^* = b\) |
| Origin at 0,1/2,z | \(a^* = (2a - b - c)/3\) \(b^* = (-a + 2b - c)/3\) |

| Along \([1,1,1]\) | p6'm'm | \(a^* = (2a - b - c)/3\) \(b^* = (-a + 2b - c)/3\) |
| Origin at \(x,x,x\) | \(a^* = c/2\) \(b^* = (-a + b)/2\) |

| Along \([1,1,0]\) | \(p_{2a^*}2mm\) |
| \(a^* = (2a - b - c)/3\) \(b^* = (-a + 2b - c)/3\) |
| Origin at \(x,x,1/4\) | |
Origin at center (m\(\overline{3}1\)')

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad z \leq \min(x, 1/2-x, y, 1/2-y)\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/4,1/4,1/4\]

Symmetry Operations

For 1 + set

\begin{align*}
(1) & \quad 1 \\
(1\!0,0,0) & \quad (2) \quad 0,0,z \quad (2\!z,0,0) \\
 & \quad (3) \quad 0,y,0 \quad (2\!y,0,0) \\
 & \quad (4) \quad 2 \times 0,0 \quad (2\!,0,0) \\
(5) & \quad 3^+ x,x,x \\
(3_{xyz}\!0,0,0) & \quad (6) \quad 3^+ \overline{x},\overline{x},\overline{x} \\
 & \quad (3_{xyz}\!^{-1}0,0,0) \\
 & \quad (7) \quad 3^+ x,x,\overline{x} \\
 & \quad (3_{xyz}\!^{-1}0,0,0) \\
 & \quad (8) \quad 3^+ \overline{x},\overline{x},x \\
 & \quad (3_{xyz}\!^{-1}0,0,0) \\
(9) & \quad 3^- x,x,x \\
(3_{xyz}\!^{-1}0,0,0) & \quad (10) \quad 3^- \overline{x},\overline{x},\overline{x} \\
 & \quad (3_{xyz}\!0,0,0) \\
 & \quad (11) \quad 3^- x,\overline{x},\overline{x} \\
 & \quad (3_{xyz}\!0,0,0) \\
 & \quad (12) \quad 3^- \overline{x},x,\overline{x} \\
 & \quad (3_{xyz}\!0,0,0)
\end{align*}
Continued 223.2.1607 Pm3n1'

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25); 1'.

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Continued 223.2.1607 Pm3n1'

48  I  11'

(1) x,y,z [0,0,0]  
(2) x,y,z [0,0,0]  
(3) x,y,z [0,0,0]  
(4) x,y,z [0,0,0]

(5) z,x,y [0,0,0]  
(6) z,x,y [0,0,0]  
(7) z,x,y [0,0,0]  
(8) z,x,y [0,0,0]

(9) y,z,x [0,0,0]  
(10) y,z,x [0,0,0]  
(11) y,z,x [0,0,0]  
(12) y,z,x [0,0,0]

(13) y+1/2,x+1/2,z+1/2 [0,0,0]  
(14) y+1/2,x+1/2,z+1/2 [0,0,0]  
(15) y+1/2,x+1/2,z+1/2 [0,0,0]  
(16) y+1/2,x+1/2,z+1/2 [0,0,0]

(17) x+1/2,z+1/2,y+1/2 [0,0,0]  
(18) x+1/2,z+1/2,y+1/2 [0,0,0]  
(19) x+1/2,z+1/2,y+1/2 [0,0,0]  
(20) x+1/2,z+1/2,y+1/2 [0,0,0]

(21) z+1/2,y+1/2,x+1/2 [0,0,0]  
(22) z+1/2,y+1/2,x+1/2 [0,0,0]  
(23) z+1/2,y+1/2,x+1/2 [0,0,0]  
(24) z+1/2,y+1/2,x+1/2 [0,0,0]

(25) x,y,z [0,0,0]  
(26) x,y,z [0,0,0]  
(27) x,y,z [0,0,0]  
(28) x,y,z [0,0,0]

(29) z,x,y [0,0,0]  
(30) z,x,y [0,0,0]  
(31) z,x,y [0,0,0]  
(32) z,x,y [0,0,0]

(33) y,z,x [0,0,0]  
(34) y,z,x [0,0,0]  
(35) y,z,x [0,0,0]  
(36) y,z,x [0,0,0]

(37) y+1/2,x+1/2,z+1/2 [0,0,0]  
(38) y+1/2,x+1/2,z+1/2 [0,0,0]  
(39) y+1/2,x+1/2,z+1/2 [0,0,0]  
(40) y+1/2,x+1/2,z+1/2 [0,0,0]

(41) x+1/2,z+1/2,y+1/2 [0,0,0]  
(42) x+1/2,z+1/2,y+1/2 [0,0,0]  
(43) x+1/2,z+1/2,y+1/2 [0,0,0]  
(44) x+1/2,z+1/2,y+1/2 [0,0,0]

(45) z+1/2,y+1/2,x+1/2 [0,0,0]  
(46) z+1/2,y+1/2,x+1/2 [0,0,0]  
(47) z+1/2,y+1/2,x+1/2 [0,0,0]  
(48) z+1/2,y+1/2,x+1/2 [0,0,0]

24 k m..1' 0,y,z [0,0,0]  
0,y,z [0,0,0]  
0,y,z [0,0,0]  
0,y,z [0,0,0]

z,0,y [0,0,0]  
z,0,y [0,0,0]  
z,0,y [0,0,0]  
z,0,y [0,0,0]

y,z,0 [0,0,0]  
y,z,0 [0,0,0]  
y,z,0 [0,0,0]  
y,z,0 [0,0,0]

223.2.1607 - 3 - 3677
<table>
<thead>
<tr>
<th></th>
<th>d</th>
<th>m.21'</th>
<th>1/4,1/2,0 [0,0,0]</th>
<th>3/4,1/2,0 [0,0,0]</th>
<th>0,1/4,1/2 [0,0,0]</th>
</tr>
</thead>
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<tr>
<td></td>
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<td>0,3/4,1/2 [0,0,0]</td>
<td>1/2,0,1/4 [0,0,0]</td>
<td>1/2,0,3/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>c</td>
<td>m.21'</td>
<td>1/4,0,1/2 [0,0,0]</td>
<td>3/4,0,1/2 [0,0,0]</td>
<td>1/2,1/4,0 [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>1/2,3/4,0 [0,0,0]</td>
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<td>0,1/2,3/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td>b</td>
<td>mmm..1'</td>
<td>0,1/2,1/2 [0,0,0]</td>
<td>1/2,0,1/2 [0,0,0]</td>
<td>1/2,1/2,0 [0,0,0]</td>
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<td>0,0,1/2 [0,0,0]</td>
<td></td>
</tr>
<tr>
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<td></td>
<td>m3.1'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4mm1'  
\( \mathbf{a}^* = \mathbf{a} \quad \mathbf{b}^* = \mathbf{b} \)  
Origin at 0,1/2,z

Along [1,1,1] p6mm1'  
\( \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \quad \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3 \)  
Origin at x,x,x

Along [1,1,0] p2mm1'  
\( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2 \)  
Origin at x,x,0
Origin at center (m\(^3\)\(^n\))

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad z \leq \min(x, 1/2-x, y, 1/2-y)\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 0,1/2,0 \quad 1/4,1/4,1/4\]

Symmetry Operations

\begin{align*}
(1) & \quad 1 \\
& \quad (1|0,0,0) \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2z|0,0,0) \\
(3) & \quad 2 \quad 0,y,0 \\
& \quad (2y|0,0,0) \\
(4) & \quad 2 \quad x,0,0 \\
& \quad (2x|0,0,0) \\
(5) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}|0,0,0) \\
(6) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(7) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(8) & \quad 3^+ \quad x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(9) & \quad 3^{-}\quad x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(10) & \quad 3^{-}\quad x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(11) & \quad 3^{-}\quad x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
(12) & \quad 3^{-}\quad x,x,x \\
& \quad (3_{xyz}^{-1}|0,0,0) \\
\end{align*}
Continued

223.3.1608 Pm$^{3}$n

13) $2^{'} (1/2,1/2,0) \ x,x,1/4$
   $\begin{cases} \text{continued} \\ 3 \end{cases}$

17) $4^{'} (1/2,0,0) \ x,1/2,0$
   $\begin{cases} \text{continued} \\ 4 \end{cases}$

21) $4^{'} (0,1/2,0) \ 1/2,y,0$
   $\begin{cases} \text{continued} \\ 5 \end{cases}$

25) $1^{'} 0,0,0$
   $\begin{cases} \text{continued} \\ 6 \end{cases}$

29) $3^{'} x,x,x; 0,0,0$
   $\begin{cases} \text{continued} \\ 7 \end{cases}$

33) $3^{'} x,x,x; 0,0,0$
   $\begin{cases} \text{continued} \\ 8 \end{cases}$

37) $c (0,0,1/2) \ x+1/2,\bar{z},z$
   $\begin{cases} \text{continued} \\ 9 \end{cases}$

41) $4^{'} x,0,1/2; 1/4,0,1/2$
   $\begin{cases} \text{continued} \\ 10 \end{cases}$

45) $4^{'} 0,y,1/2; 0,1/4,1/2$
   $\begin{cases} \text{continued} \\ 11 \end{cases}$

Generators selected

(1): $t(1,0,0); t(0,1,0); t(0,0,1)$; (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48 1 1

(1) $x,y,z [u,v,w]$
   (2) $\bar{x},\bar{y},\bar{z} [u,\bar{v},w]$
   (3) $x,y,z [u,v,w]$
   (4) $x,\bar{y},\bar{z} [u,\bar{v},w]$

(5) $z,x,y [w,u,v]$
   (6) $z,\bar{x},\bar{y} [w,\bar{u},v]$
   (7) $\bar{z},x,y [w,u,\bar{v}]$
   (8) $\bar{z},x,y [w,u,v]$

(9) $y,z,x [v,w,u]$
   (10) $\bar{y},z,\bar{x} [v,w,u]$
   (11) $y,z,\bar{x} [v,w,u]$
   (12) $\bar{y},z,x [\bar{v},w,u]$

(13) $y+1/2,x+1/2,z+1/2 [v,\bar{u},w]$ (14) $y+1/2,x+1/2,z+1/2 [v,u,w]$ (15) $y+1/2,x+1/2,z+1/2 [v,u,\bar{w}]$
   (16) $y+1/2,x+1/2,z+1/2 [v,\bar{u},\bar{w}]$

(17) $x+1/2,z+1/2,y+1/2 [u,\bar{w},v]$ (18) $x+1/2,z+1/2,y+1/2 [u,w,\bar{v}]$
   (19) $x+1/2,z+1/2,y+1/2 [u,w,v]$ (20) $x+1/2,z+1/2,y+1/2 [u,\bar{w},v]$

(21) $z+1/2,y+1/2,x+1/2 [\bar{w},\bar{v},u]$ (22) $z+1/2,y+1/2,x+1/2 [\bar{w},\bar{u},v]$ (23) $\bar{z}+1/2,y+1/2,x+1/2 [\bar{w},\bar{v},u]$
   (24) $\bar{z}+1/2,y+1/2,x+1/2 [\bar{w},\bar{u},v]$

(25) $\bar{x},\bar{y},\bar{z} [u,\bar{v},w]$ (26) $x,\bar{y},\bar{z} [u,\bar{v},w]$ (27) $x,\bar{y},\bar{z} [u,\bar{v},w]$ (28) $x,\bar{y},\bar{z} [u,\bar{v},w]$

(29) $\bar{z},x,y [w,\bar{u},v]$ (30) $\bar{z},x,y [w,u,\bar{v}]$
   (31) $\bar{z},x,y [w,u,v]$ (32) $\bar{z},x,y [w,u,v]$

(33) $y,z,\bar{x} [v,\bar{w},u]$ (34) $y,z,\bar{x} [v,w,u]$ (35) $\bar{y},\bar{z},\bar{x} [\bar{w},w,u]$ (36) $\bar{y},\bar{z},\bar{x} [\bar{w},w,u]$

223.3.1608 - 2 - 3681
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</tbody>
</table>

**Symmetry of Special Projections**

- Along [0,0,1] `p4'm'm`
  - `a` = `a`  `b` = `b`
  - `Origin at 0,1/2,z`
- Along [1,1,1] `p6mm`
  - `a` = `(2a - b - c)/3`  `b` = `(-a + 2b - c)/3`
  - `Origin at x,x,x`
- Along [1,1,0] `p2mm`
  - `a` = `c/2`  `b` = `(-a + b)/2`
  - `Origin at x,x,0`
Origin at center (m\bar{3})

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq \frac{1}{4}; \quad z \leq \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y) \]

Vertices

\[ 0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad 0,\frac{1}{2},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4} \]

Symmetry Operations

(1)\quad 1
(2)\quad 2 \quad 0,0,0 \quad (2_z|0,0,0)
(3)\quad 2 \quad 0,0,0 \quad (2_y|0,0,0)
(4)\quad 2 \quad x,0,0 \quad (2_x|0,0,0)

(5)\quad 3^+ \quad x,x,x \quad (3_{xyz}|0,0,0)
(6)\quad 3^+ \quad x,x,x \quad (3_{xyz}^{-1}|0,0,0)
(7)\quad 3^+ \quad x,x,x \quad (3_{xyz}^{-1}|0,0,0)
(8)\quad 3^+ \quad \bar{x},\bar{x},\bar{x} \quad (3_{xyz}^{-1}|0,0,0)

(9)\quad 3^- \quad x,x,x \quad (3_{xyz}^{-1}|0,0,0)
(10)\quad 3^- \quad x,x,x \quad (3_{xyz}|0,0,0)
(11)\quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (3_{xyz}|0,0,0)
(12)\quad 3^- \quad \bar{x},\bar{x},\bar{x} \quad (3_{xyz}|0,0,0)
Continued

| (13) | 2' (1/2,1/2,0) | x,x,1/4 |
| (14) | 2' x,x+1/2,1/4 |
| (15) | 4' (0,0,1/2) | 1/2,0,z |
| (16) | 4' (0,0,1/2) | 0,1/2,z |
| (17) | 4' (1/2,0,0) | x,1/2,0 |
| (18) | 2' (0,1/2,1/2) | 1/4,y,y |
| (19) | 2' 1/4,y+1/2,y |
| (20) | 4' (1/2,0,0) | x,0,1/2 |
| (21) | 4' (0,1/2,0) | 1/2,y,0 |
| (22) | 2' (1/2,1/2,1/2) | x,1/4,x |
| (23) | 4' (0,1/2,0) | 0,y,1/2 |
| (24) | 2' x+1/2,1/4,x |
| (25) | 1,0,0 |
| (1) | 0,0,0 |
| (26) | m x,y,0 |
| (27) | m x,0,z |
| (28) | m y,z,0 |
| (29) | 3' x,x,x; 0,0,0 |
| (30) | 3' x,x,x; 0,0,0 |
| (31) | 3' x,x,x; 0,0,0 |
| (32) | 3' x,x,x; 0,0,0 |
| (33) | 3' x,x,x; 0,0,0 |
| (34) | 3' x,x,x; 0,0,0 |
| (35) | 3' x,x,x; 0,0,0 |
| (36) | 3' x,x,x; 0,0,0 |
| (37) | c' (0,0,1/2) |
| (38) | n' (1/2,1/2,1/2) |
| (39) | 4' 0,1/2,z; 0,1/2,1/4 |
| (40) | 4' 1/2,0,z; 1/2,0,1/4 |
| (41) | 4' x,0,1/2; 1/4,0,1/2 |
| (42) | a' (1/2,0,0) |
| (43) | n' (1/2,1/2,1/2) |
| (44) | 4' x,1/2,0; 1/4,1/2,0 |
| (45) | 4' 0,y,1/2; 0,1/4,1/2 |
| (46) | b' (0,1/2,0) |
| (47) | 4' 1/2,y,0; 1/2,1/4,0 |
| (48) | n' (1/2,1/2,1/2) |

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

48 1 1

| (1) | x,y,z [u,v,w] |
| (2) | x,y,z [u,v,w] |
| (3) | x,y,z [u,v,w] |
| (4) | x,y,z [u,v,w] |
| (5) | z,x,y [w,u,v] |
| (6) | z,x,y [w,u,v] |
| (7) | z,x,y [w,u,v] |
| (8) | z,x,y [w,u,v] |
| (9) | y,z,x [v,w,u] |
| (10) | y,z,x [v,w,u] |
| (11) | y,z,x [v,w,u] |
| (12) | y,z,x [v,w,u] |
| (13) | y+1/2,x+1/2,z+1/2 [v,u,w] |
| (14) | y+1/2,x+1/2,z+1/2 [v,u,w] |
| (15) | y+1/2,x+1/2,z+1/2 [v,u,w] |
| (16) | y+1/2,x+1/2,z+1/2 [v,u,w] |
| (17) | x+1/2,z+1/2,y+1/2 [u,w,v] |
| (18) | x+1/2,z+1/2,y+1/2 [u,w,v] |
| (19) | x+1/2,z+1/2,y+1/2 [u,w,v] |
| (20) | x+1/2,z+1/2,y+1/2 [u,w,v] |
| (21) | z+1/2,y+1/2,x+1/2 [w,v,u] |
| (22) | z+1/2,y+1/2,x+1/2 [w,v,u] |
| (23) | z+1/2,y+1/2,x+1/2 [w,v,u] |
| (24) | z+1/2,y+1/2,x+1/2 [w,v,u] |
| (25) | x,y,z [u,v,w] |
| (26) | x,y,z [u,v,w] |
| (27) | x,y,z [u,v,w] |
| (28) | x,y,z [u,v,w] |
| (29) | z,x,y [w,u,v] |
| (30) | z,x,y [w,u,v] |
| (31) | z,x,y [w,u,v] |
| (32) | z,x,y [w,u,v] |
| (33) | y,z,x [v,w,u] |
| (34) | y,z,x [v,w,u] |
| (35) | y,z,x [v,w,u] |
| (36) | y,z,x [v,w,u] |
(37) \( y+1/2, x+1/2, z+1/2 \) \([v,u,w]\) (38) \( y+1/2, x+1/2, z+1/2 \) \([v,u,w]\) (39) \( y+1/2, x+1/2, z+1/2 \) \([v,u,w]\) (40) \( y+1/2, x+1/2, z+1/2 \) \([v,u,w]\) (41) \( x+1/2, y+1/2, z+1/2 \) \([w,v,\bar{u},\bar{v}]\) (42) \( x+1/2, y+1/2, z+1/2 \) \([u,\bar{v},w]\) (43) \( x+1/2, y+1/2, z+1/2 \) \([u,\bar{v},w]\) (44) \( x+1/2, y+1/2, z+1/2 \) \([u,\bar{v},w]\) (45) \( z+1/2, y+1/2, x+1/2 \) \([w,v,u]\) (46) \( z+1/2, y+1/2, x+1/2 \) \([w,v,u]\) (47) \( z+1/2, y+1/2, x+1/2 \) \([w,v,u]\) (48) \( z+1/2, y+1/2, x+1/2 \) \([w,v,u]\)

24 k m.. 0,y,z [u,0,0] 0,y,z [u,0,0] 0,y,z [u,0,0] 
24 j .2'

1/4,y,y+1/2 [u,v,v] 3/4,y,y+1/2 [u,v,v] 3/4,y,y+1/2 [u,v,v] 1/4,y,y+1/2 [u,v,v]

y+1/2,1/4, y [v,u,v] y+1/2,1/4, y [v,u,v] y+1/2,1/4, y [v,u,v] y+1/2,1/4, y [v,u,v]

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16 i .3. x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]

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x,x,x [u,u,u] x,x,x [u,u,u] x,x,x [u,u,u]

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12 h mm2.. x,1/2,0 [0,0,0] x,1/2,0 [0,0,0] 0,x,1/2 [0,0,0] 0,x,1/2 [0,0,0]

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x+1/2,1/2,0 [0,0,0] x+1/2,1/2,0 [0,0,0] 1/2,0,x+1/2 [0,0,0] 1/2,0,x+1/2 [0,0,0]
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<tr>
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<td>m3.</td>
<td>m3.</td>
<td>m3.</td>
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**Symmetry of Special Projections**

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<th>Symmetry</th>
<th>Origin</th>
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<td>Along [0,0,1]</td>
<td>p4mm1'</td>
<td>0,1/2,z</td>
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<tr>
<td><strong>a</strong> = a</td>
<td><strong>a</strong> = (2a - b - c)/3</td>
<td>Origin at 0,1/2,z</td>
</tr>
<tr>
<td><strong>b</strong> = b</td>
<td><strong>b</strong> = (-a + 2b - c)/3</td>
<td></td>
</tr>
<tr>
<td>Along [1,1,1]</td>
<td>p6'mm'</td>
<td>x,x,x</td>
</tr>
<tr>
<td><strong>a</strong> = c/2</td>
<td><strong>a</strong> = c/2</td>
<td>Origin at x,x,x</td>
</tr>
<tr>
<td><strong>b</strong> = (-a + b)/2</td>
<td><strong>b</strong> = (-a + b)/2</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (m'3')

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4;  
z ≤ min(x, 1/2-x, y, 1/2-y)

Vertices  
0,0,0  1/2,0,0  1/2,1/2,0  0,1/2,0  1/4,1/4,1/4

Symmetry Operations

(1) 1
(1) 0,0,0
(1) 0,0,0

(2) 2 0,0,z
(2) 0,0,0
(2) 0,0,0

(3) 2 0,y,0
(3) 0,0,0
(3) 0,0,0

(4) 2 x,0,0
(4) 0,0,0
(4) 0,0,0

(5) 3' x,x,x
(3) x,y,x
(3) x,y,x

(6) 3' x,x,x
(3) x,y,x
(3) x,y,x

(7) 3' x,x,x
(3) x,y,x
(3) x,y,x

(8) 3' x,x,x
(3) x,y,x
(3) x,y,x

(9) 3' x,x,x
(3) x,y,x
(3) x,y,x

(10) 3' x,x,x
(3) x,y,x
(3) x,y,x

(11) 3' x,x,x
(3) x,y,x
(3) x,y,x

(12) 3' x,x,x
(3) x,y,x
(3) x,y,x
Continued

| (13) 2 (1/2,1/2,0) x,x,1/4 | (14) 2 x,x+1/2,1/4 | (15) 4' (0,0,1/2) 1/2,0,z | (16) 4' (0,0,1/2) 0,1/2,z |
| (2y) 1/2,1/2,1/2 | (2y) 1/2,1/2,1/2 | (4z) 1/2,1/2,1/2 | (4z) 1/2,1/2,1/2 |
| (17) 4' (1/2,0,0) x,1/2,0 | (18) 2 (0,1/2,1/2) 1/4,y,y | (19) 2 1/4,y+1/2,y | (20) 4' (1/2,0,0) x,0,1/2 |
| (4x) 1/2,1/2,1/2 | (2y) 1/2,1/2,1/2 | (2y) 1/2,1/2,1/2 | (4x) 1/2,1/2,1/2 |
| (21) 4' (0,1/2,0) 1/2,y,0 | (22) 2 (1/2,0,1/2) x,1/4,x | (23) 4' (0,1/2,0) 0,y,1/2 | (24) 2 x+1/2,1/4,x |
| (4y) 1/2,1/2,1/2 | (2y) 1/2,1/2,1/2 | (4y) 1/2,1/2,1/2 | (2x) 1/2,1/2,1/2 |
| (25) t' 0,0,0 | (26) m' x,y,0 | (27) m' x,0,z | (28) m' 0,y,z |
| (1 0,0,0)' | (m_x 0,0,0)' | (m_y 0,0,0)' | (m_y 0,0,0)' |
| (29) 3++ x,x,x; 0,0,0 | (30) 3++ x,x,x; 0,0,0 | (31) 3++ x,x,x; 0,0,0 | (32) 3++ x,x,x; 0,0,0 |
| (3xyz 0,0,0)' | (3xyz 0,0,0)' | (3xyz 0,0,0)' | (3xyz 0,0,0)' |
| (33) 3+ x,x,x; 0,0,0 | (34) 3+ x,x,x; 0,0,0 | (35) 3+ x,x,x; 0,0,0 | (36) 3+ x,x,x; 0,0,0 |
| (3xyz 0,0,0)' | (3xyz 0,0,0)' | (3xyz 0,0,0)' | (3xyz 0,0,0)' |
| (37) c' (0,0,1/2) x+1/2,z,z | (38) n' (1/2,1/2,1/2) x,x,z | (39) 4'' x,x,x; 0,1/2,z; 0,1/2,1/4 | (40) 4'' 1/2,0,z; 1/2,0,1/4 |
| (m_y 1/2,1/2,12)' | (m_y 1/2,1/2,12)' | (4z) 1/2,1/2,12)' | (4z) 1/2,1/2,12)' |
| (41) 4+ x,0,1/2; 1/4,0,1/2 | (42) a' (1/2,0,0) x,y+1/2,y | (43) n' (1/2,1/2,1/2) x,y,y | (44) 4' x,1/2,0; 1/4,1/2,0 |
| (4y) 1/2,1/2,12)' | (m_y 1/2,1/2,12)' | (m_y 1/2,1/2,12)' | (4x) 1/2,1/2,12)' |
| (45) 4+ x,0,1/2; 0,1/4,1/2 | (46) b' (0,1/2,0) x+1/2,y,x | (47) 4' x,x,x; 1/2,0,y; 1/2,1/4,0 | (48) n' (1/2,1/2,1/2) x,y,x |
| (4y) 1/2,1/2,12)' | (m_y 1/2,1/2,12)' | (4y) 1/2,1/2,12)' | (m_y 1/2,1/2,12)' |

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); (2): (3); (5): (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

| 48 | 1 |
| 1 | (1) x,y,z [u,v,w] (2) x+y,z [u,v,w] (3) x,y,z [u,v,w] (4) x+y,z [u,v,w] |
| 5 | (5) z,x,y [w,u,v] (6) z,x,y [w,u,v] (7) z,x,y [w,u,v] (8) z,x,y [w,u,v] |
| 9 | (9) y,z,x [v,w,u] (10) y,z,x [v,w,u] (11) y,z,x [v,w,u] (12) y,z,x [v,w,u] |
| 13 | (13) y+1/2,x+1/2,z+1/2 [v,u,w] (14) y+1/2,x+1/2,z+1/2 [v,u,w] (15) y+1/2,x+1/2,z+1/2 [v,u,w] (16) y+1/2,x+1/2,z+1/2 [v,u,w] |
| 17 | (17) x+1/2,z+1/2,y+1/2 [u,w,v] (18) x+1/2,z+1/2,y+1/2 [u,w,v] (19) x+1/2,z+1/2,y+1/2 [u,w,v] (20) x+1/2,z+1/2,y+1/2 [u,w,v] |
| 21 | (21) z+1/2,y+1/2,x+1/2 [w,v,u] (22) z+1/2,y+1/2,x+1/2 [w,v,u] (23) z+1/2,y+1/2,x+1/2 [w,v,u] (24) z+1/2,y+1/2,x+1/2 [w,v,u] |
| 25 | (25) x,y,z [u,v,w] (26) x,y,z [u,v,w] (27) x,y,z [u,v,w] (28) x,y,z [u,v,w] |
| 29 | (29) z,x,y [w,u,v] (30) z,x,y [w,u,v] (31) z,x,y [w,u,v] (32) z,x,y [w,u,v] |
| 33 | (33) y,z,x [v,w,u] (34) y,z,x [v,w,u] (35) y,z,x [v,w,u] (36) y,z,x [v,w,u] |
Continued

$$y + 1/2, x + 1/2, z + 1/2$$

<table>
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<tr>
<th>24</th>
<th>k</th>
<th>m'..</th>
<th>0, y, z [0, v, w]</th>
<th>0, y, z [0, v, w]</th>
<th>0, y, z [0, v, w]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, y, z [0, v, w]</td>
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<td>0, y, z [0, v, w]</td>
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<tr>
<td>z, 0, y [w, 0, v]</td>
<td>z, 0, y [w, 0, v]</td>
<td>z, 0, y [w, 0, v]</td>
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<tr>
<td>y, z, 0 [v, w, 0]</td>
<td>y, z, 0 [v, w, 0]</td>
<td>y, z, 0 [v, w, 0]</td>
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<tr>
<td>y + 1/2, 1/2, z + 1/2 [v, 0, w]</td>
<td>y + 1/2, 1/2, z + 1/2 [v, 0, w]</td>
<td>y + 1/2, 1/2, z + 1/2 [v, 0, w]</td>
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<tr>
<td>1/2, z + 1/2, y + 1/2 [0, w, v]</td>
<td>1/2, z + 1/2, y + 1/2 [0, w, v]</td>
<td>1/2, z + 1/2, y + 1/2 [0, w, v]</td>
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<tr>
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<td>z + 1/2, y + 1/2, 1/2 [w, v, 0]</td>
<td>z + 1/2, y + 1/2, 1/2 [w, v, 0]</td>
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<table>
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<th>24</th>
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<tr>
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<td>3/4, y, y + 1/2 [0, v, v]</td>
<td>3/4, y, y + 1/2 [0, v, v]</td>
</tr>
<tr>
<td>y + 1/2, 1/4, y [v, 0, v]</td>
<td>y + 1/2, 3/4, y [v, 0, v]</td>
<td>y + 1/2, 1/4, y [v, 0, v]</td>
</tr>
<tr>
<td>y, y + 1/2, 1/4 [v, v, 0]</td>
<td>y, y + 1/2, 3/4 [v, v, 0]</td>
<td>y, y + 1/2, 1/4 [v, v, 0]</td>
</tr>
<tr>
<td>3/4, y, y + 1/2 [0, v, v]</td>
<td>1/4, y, y + 1/2 [0, v, v]</td>
<td>3/4, y, y + 1/2 [0, v, v]</td>
</tr>
<tr>
<td>y + 1/2, 3/4, y [v, 0, v]</td>
<td>y + 1/2, 1/4, y [v, 0, v]</td>
<td>y + 1/2, 3/4, y [v, 0, v]</td>
</tr>
<tr>
<td>y, y + 1/2, 3/4 [v, v, 0]</td>
<td>y, y + 1/2, 1/4 [v, v, 0]</td>
<td>y, y + 1/2, 3/4 [v, v, 0]</td>
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<tr>
<th>16</th>
<th>i</th>
<th>.. .3</th>
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<tr>
<td>x, x, x [u, u, u]</td>
<td>x, x, x [u, u, u]</td>
<td>x, x, x [u, u, u]</td>
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<td>x + 1/2, x + 1/2, x + 1/2 [u, u, u]</td>
<td>x + 1/2, x + 1/2, x + 1/2 [u, u, u]</td>
<td>x + 1/2, x + 1/2, x + 1/2 [u, u, u]</td>
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<td>x + 1/2, x + 1/2, x + 1/2 [u, u, u]</td>
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<td>x + 1/2, x + 1/2, x + 1/2 [u, u, u]</td>
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<td>x + 1/2, x + 1/2, x + 1/2 [u, u, u]</td>
<td>x + 1/2, x + 1/2, x + 1/2 [u, u, u]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>12</th>
<th>h</th>
<th>m' m'2..</th>
<th>x, 1/2, 0 [u, 0, 0]</th>
<th>0, x, 1/2 [0, u, 0]</th>
<th>0, x, 1/2 [0, u, 0]</th>
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<tbody>
<tr>
<td>x, 1/2, 0 [u, 0, 0]</td>
<td>0, x, 1/2 [0, u, 0]</td>
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</tr>
<tr>
<td>1/2, 0, x [0, 0, u]</td>
<td>0, x, 1/2 [0, u, 0]</td>
<td>0, x, 1/2 [0, u, 0]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>x + 1/2, 1/2, 0 [u, 0, 0]</td>
<td>1/2, 0, x + 1/2 [0, 0, u]</td>
<td>1/2, 0, x + 1/2 [0, 0, u]</td>
<td></td>
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<td></td>
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</tbody>
</table>

223.5.1610 - 3 - 3690
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4m'm'</th>
<th>Along [1,1,1]</th>
<th>p6m'm'</th>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = a )</td>
<td>( b^* = b )</td>
<td>( a^* = (2a - b - c)/3 )</td>
<td>( b^* = (-a + 2b - c)/3 )</td>
<td>( a^* = (-a + b)/2 )</td>
<td>( b^* = c/2 )</td>
</tr>
<tr>
<td>Origin at 0,1/2,z</td>
<td>Origin at x,x,x</td>
<td>Origin at x,x,0</td>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| 12 | g | m'm'2.. x,0,1/2 [u,0,0] | \( x,0,1/2 [u,0,0] \) | 1/2,0 [0,u,0] | 1/2,0 [0,u,0] |
| 0,1/2,x [0,0,u] | 0,1/2,x [0,0,u] | 1/2,0+1/2,0 [0,u,0] | 1/2,0+1/2,0 [0,u,0] |
| x+1/2,0,1/2 [u,0,0] | x+1/2,0,1/2 [u,0,0] | 0,1/2,x+1/2 [0,u,0] | 0,1/2,x+1/2 [0,u,0] |

| 12 | f | m'm'2.. x,0,0 [u,0,0] | \( x,0,0 [u,0,0] \) | 0,x,0 [0,u,0] | 0,x,0 [0,u,0] |
| 0,0,x [0,0,u] | 0,0,x [0,0,u] | 1/2,0+1/2,1/2 [0,u,0] | 1/2,0+1/2,1/2 [0,u,0] |
| x+1/2,1/2,1/2 [u,0,0] | x+1/2,1/2,1/2 [u,0,0] | 1/2,1/2,x+1/2 [0,u,0] | 1/2,1/2,x+1/2 [0,u,0] |

| 8 | e | .32 | 1/4,1/4,1/4 [0,0,0] | 3/4,3/4,1/4 [0,0,0] | 3/4,3/4,1/4 [0,0,0] | 3/4,3/4,1/4 [0,0,0] |
| 3/4,3/4,3/4 [0,0,0] | 3/4,1/4,1/4 [0,0,0] | 1/4,3/4,1/4 [0,0,0] | 3/4,1/4,1/4 [0,0,0] |

| 6 | d | \( \bar{4}m'.2 \) | 1/4,1/2,0 [0,0,0] | 3/4,1/2,0 [0,0,0] | 0,1/4,1/2 [0,0,0] |
| 0,3/4,1/2 [0,0,0] | 0,3/4,1/2 [0,0,0] | 1/2,0,1/4 [0,0,0] | 1/2,0,1/4 [0,0,0] |

| 6 | c | \( \bar{4}m'.2 \) | 1/4,0,1/2 [0,0,0] | 3/4,0,1/2 [0,0,0] | 1/2,1/4,0 [0,0,0] |
| 1/2,3/4,0 [0,0,0] | 1/2,3/4,0 [0,0,0] | 0,1/2,1/4 [0,0,0] | 0,1/2,3/4 [0,0,0] |

| 6 | b | m'm'm'.. | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] |
| 0,1/2,0 [0,0,0] | 0,1/2,0 [0,0,0] | 1/2,0,0 [0,0,0] | 0,0,1/2 [0,0,0] |

| 2 | a | m'3'.. | 0,0,0 [0,0,0] | 1/2,1/2,1/2 [0,0,0] | 1/2,1/2,1/2 [0,0,0] |
Origin at $\bar{4}3m$, at $-1/4,-1/4,-1/4$ from center ($\bar{3}m$)

Asymmetric unit

$0 \leq x \leq 1/2$; $0 \leq y \leq 1/2$; $-1/4 \leq z \leq 1/4$; $y \leq x$; $\max(x-1/2,-y) \leq z \leq \min(1/2-x,y)$

Vertices

0,0,0 1/2,0,0 1/2,1/2,0 1/4,1/4,1/4 1/4,1/4,-1/4

Symmetry Operations

1 2 0,0,z (2) 0,y,0 (3) 2 x,0,0 (4) 2 x,0,0

$0,0,0$ $0,0,0$ $0,0,0$ $0,0,0$

$2,0,0$ $2,0,0$ $2,0,0$ $2,0,0$

$3_x^+ x,x,x$ $3_y x,x,x$ $3_z x,x,x$ $3_x^+ x,x,x$

$(3_{xyz}|0,0,0)$ $(3_{xyz}^{-1}|0,0,0)$ $(3_{xyz}^{-1}|0,0,0)$ $(3_{xyz}^{-1}|0,0,0)$

$3_x^+ x,x,x$ $3_y x,x,x$ $3_z x,x,x$ $3_x^+ x,x,x$

$(3_{xyz}^{-1}|0,0,0)$ $(3_{xyz}^{-1}|0,0,0)$ $(3_{xyz}^{-1}|0,0,0)$ $(3_{xyz}^{-1}|0,0,0)$
Continued

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).</th>
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<tbody>
<tr>
<td>Positions</td>
<td>Coordinates</td>
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<tr>
<td>Multiplicity,</td>
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<tr>
<td>Wyckoff letter,</td>
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<td>Site Symmetry.</td>
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<table>
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<tbody>
<tr>
<td>(1)</td>
<td>x,y,z [u,v,w]</td>
</tr>
<tr>
<td>(2)</td>
<td>\bar{x},\bar{y},z [\bar{u},\bar{v},w]</td>
</tr>
<tr>
<td>(3)</td>
<td>\bar{x},y,\bar{z} [\bar{u},v,w]</td>
</tr>
<tr>
<td>(4)</td>
<td>x,\bar{y},\bar{z} [u,\bar{v},w]</td>
</tr>
<tr>
<td>(5)</td>
<td>z,x,y [w,u,v]</td>
</tr>
<tr>
<td>(6)</td>
<td>\bar{z},\bar{x},\bar{y} [w,\bar{u},\bar{v}]</td>
</tr>
<tr>
<td>(7)</td>
<td>\bar{z},x,y [w,\bar{u},v]</td>
</tr>
<tr>
<td>(8)</td>
<td>\bar{z},x,\bar{y} [w,\bar{u},v]</td>
</tr>
<tr>
<td>(9)</td>
<td>y,z,x [v,w,u]</td>
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<tr>
<td>(10)</td>
<td>\bar{y},\bar{x},z [v,\bar{w},u]</td>
</tr>
<tr>
<td>(11)</td>
<td>\bar{y},z,\bar{x} [v,\bar{w},u]</td>
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<tr>
<td>(12)</td>
<td>\bar{y},z,x [v,\bar{w},u]</td>
</tr>
<tr>
<td>(13)</td>
<td>y+1/2,x+1/2,z+1/2 [v,w,u]</td>
</tr>
<tr>
<td>(14)</td>
<td>\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2 [\bar{v},\bar{w},\bar{u}]</td>
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<td>(15)</td>
<td>y+1/2,x+1/2,z+1/2 [v,w,u]</td>
</tr>
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<td>(16)</td>
<td>\bar{y}+1/2,\bar{x}+1/2,\bar{z}+1/2 [\bar{v},\bar{w},\bar{u}]</td>
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<td>(18)</td>
<td>\bar{x}+1/2,z+1/2,y+1/2 [\bar{u},w,\bar{v}]</td>
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<td>(19)</td>
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<tr>
<td>(20)</td>
<td>\bar{x}+1/2,z+1/2,y+1/2 [\bar{u},w,\bar{v}]</td>
</tr>
<tr>
<td>(21)</td>
<td>z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(22)</td>
<td>\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [w,\bar{v},\bar{u}]</td>
</tr>
<tr>
<td>(23)</td>
<td>z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(24)</td>
<td>\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [w,\bar{v},\bar{u}]</td>
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<td>(25)</td>
<td>\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [w,\bar{v},\bar{u}]</td>
</tr>
<tr>
<td>(26)</td>
<td>z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(27)</td>
<td>\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [\bar{w},\bar{v},\bar{u}]</td>
</tr>
<tr>
<td>(28)</td>
<td>z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(29)</td>
<td>\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [w,\bar{v},\bar{u}]</td>
</tr>
<tr>
<td>(30)</td>
<td>z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(31)</td>
<td>\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [w,\bar{v},\bar{u}]</td>
</tr>
<tr>
<td>(32)</td>
<td>z+1/2,y+1/2,x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(33)</td>
<td>\bar{z}+1/2,\bar{y}+1/2,\bar{x}+1/2 [w,\bar{v},\bar{u}]</td>
</tr>
<tr>
<td>(34)</td>
<td>y+1/2,z+1/2,x+1/2 [v,w,u]</td>
</tr>
<tr>
<td>(35)</td>
<td>\bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [\bar{v},\bar{w},\bar{u}]</td>
</tr>
<tr>
<td>(36)</td>
<td>y+1/2,z+1/2,x+1/2 [v,w,u]</td>
</tr>
<tr>
<td>(37)</td>
<td>\bar{y}+1/2,\bar{z}+1/2,\bar{x}+1/2 [\bar{v},\bar{w},\bar{u}]</td>
</tr>
</tbody>
</table>

224.1.1611 - 2 - 2207
Symmetry of Special Projections

Along [0,0,1]  p4mm1'  
\( a^* = (a - b)/2 \)  \( b^* = (a + b)/2 \)  
Origin at 0,0,z

Along [1,1,1]  p6'm'm  
\( a^* = (2a - b - c)/3 \)  \( b^* = (-a + 2b - c)/3 \)  
Origin at x,x,x

Along [1,1,0]  p2mm1'  
\( a^* = (-a + b)/2 \)  \( b^* = c \)  
Origin at x,x,1/4
Origin at 4 3m1', at -1/4,-1/4,-1/4 from center (3 m1')

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad y \leq x; \quad \max(x-1/2,-y) \leq z \leq \min(1/2-x,y)\]

Vertices

\(0,0,0\)
\(1/2,0,0\)
\(1/2,1/2,0\)
\(1/4,1/4,1/4\)
\(1/4,1/4,-1/4\)

Symmetry Operations

For 1 + set

\(1\)
\(1 (1,0,0,0)\)

\(2\)
\(2 0,0,z\)
\(2_1 0,0,0\)

\(3^+\)
\(x,x,x\)
\(3_{xyz} | 0,0,0\)

\(3^-\)
\(x,x,x\)
\(3_{xyz}^{-1} | 0,0,0\)

\(10\)
\(3' x,x,x\)
\(3_{xyz} | 0,0,0\)

\(11\)
\(3' x,x,x\)
\(3_{xyz}^{-1} | 0,0,0\)
Continued

224.2.1612 Pn\textsuperscript{3}m1'

\begin{align*}
(13) & \quad 2 \ (1/2,1/2,0) \quad x,x,1/4 \\
& \quad (2_{xy}) 1/2,1/2,1/2) \\
(17) & \quad 4' \ (1/2,0,0) \quad x,1/2,0 \\
& \quad (4_{x}^{-1}) 1/2,1/2,1/2) \\
(21) & \quad 4' \ (0,1/2,0) \quad 1/2,y,0 \\
& \quad (4_{y}) 1/2,1/2,1/2) \\
(25) & \quad \overline{1} \ 1/4,1/4,1/4 \\
& \quad (1/2,1/2,12) \\
(29) & \quad 3' \ x,x,x; 1/4,1/4,1/4 \\
& \quad (3_{xyz}) 1/2,1/2,12) \\
(33) & \quad \overline{3} \ x,x,x; 1/4,1/4,1/4 \\
& \quad (3_{xyz}) 1/2,1/2,12) \\
(37) & \quad m \ x,x,z \\
& \quad (m_{yz}) 0,0,0) \\
(41) & \quad 4' \ x,0,0; 0,0,0 \\
& \quad (4_{x}) 0,0,0) \\
(45) & \quad 4' \ y,0,0; 0,0,0 \\
& \quad (4_{y}) 0,0,0) \\
(49) & \quad m \ x,y,y \\
& \quad (m_{yz}) 0,0,0) \\
(53) & \quad m \ x,z \\
& \quad (m_{yz}) 0,0,0) \\
(57) & \quad m \ x,z \\
& \quad (m_{yz}) 0,0,0) \\
(61) & \quad m \ x,y \\
& \quad (m_{yz}) 0,0,0) \\
(65) & \quad m \ x,y \\
& \quad (m_{yz}) 0,0,0) \\

& \quad \text{For 1' + set}

(1) 1' \\
(1 \ 0,0,0) \\
(5) 3' \ x,x,x \\
(3_{xyz}) 0,0,0) \\
(9) 3' \ x,x,x \\
(3_{xyz}) 0,0,0) \\
(13) 2' \ (1/2,1/2,0) \ x,x,1/4 \\
(2_{xy}) 1/2,1/2,1/2) \\
(17) 4' \ (1/2,0,0) \ x,1/2,0 \\
(4_{x}) 1/2,1/2,1/2) \\
(21) 4' \ (0,1/2,0) \ 1/2,y,0 \\
(4_{y}) 1/2,1/2,1/2) \\
(25) \overline{1} \ 1/4,1/4,1/4 \\
(1/2,1/2,12) \\
(29) 3' \ x,x,x; 1/4,1/4,1/4 \\
(3_{xyz}) 1/2,1/2,12) \\
(33) \overline{3} \ x,x,x; 1/4,1/4,1/4 \\
(3_{xyz}) 1/2,1/2,12) \\

(14) 2 \ x,x+1/2,1/4 \\
(2_{xy}) 1/2,1/2,1/2) \\
(18) 2 \ (0,1/2,1/2) \ 1/4,y,y \\
(2_{yz}) 1/2,1/2,1/2) \\
(22) 2 \ (1/2,0,1/2) \ x,1/4,x \\
(2_{yz}) 1/2,1/2,1/2) \\
(26) n' \ (1/2,1/2,0) \ x,y,1/4 \\
(2_{yz}) 1/2,1/2,1/2) \\
(30) 3' \ x-1,x+1,x; -1/4,1/4,3/4 \\
(3_{xyz}) 1/2,1/2,12) \\
(34) 3' \ x+1,x-1,x; -1/4,1/4,3/4 \\
(3_{xyz}) 1/2,1/2,12) \\
(38) m \ x,x,z \\
(3_{xyz}) 0,0,0) \\
(42) m \ x,y,y \\
(3_{xyz}) 0,0,0) \\
(46) m \ x,y,x \\
(3_{xyz}) 0,0,0) \\
(50) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(54) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(58) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(62) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(66) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(70) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(74) m \ x,z \\
(3_{xyz}) 0,0,0) \\

(15) 4' \ (0,0,1/2) \ 1/2,0,z \\
(4_{z}) 1/2,1/2,1/2) \\
(19) 2' \ 1/4,y+1/2,y \\
(2_{yz}) 1/2,1/2,1/2) \\
(23) 4' \ (0,1/2,0) \ 0,y,1/2 \\
(4_{y}) 1/2,1/2,1/2) \\
(27) n' \ (1/2,0,1/2) \ x,1/4,z \\
(2_{yz}) 1/2,1/2,1/2) \\
(31) 3' \ x,x+1,x; 1/4,3/4,-1/4 \\
(3_{xyz}) 1/2,1/2,12) \\
(35) 3' \ x,x+1,x; -1/4,3/4,1/4 \\
(3_{xyz}) 1/2,1/2,12) \\
(39) 4' \ 0,0,z; 0,0,0 \\
(4_{z}) 0,0,0) \\
(43) m \ x,y,y \\
(3_{xyz}) 0,0,0) \\
(47) 4' \ 0,y,0; 0,0,0 \\
(3_{xyz}) 0,0,0) \\
(51) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(55) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(59) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(63) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(67) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(71) m \ x,z \\
(3_{xyz}) 0,0,0) \\
(75) m \ x,z \\
(3_{xyz}) 0,0,0) \\

(16) 4' \ (0,1/2,0) \ x,0,1/2 \\
(2_{yz}) 1/2,1/2,1/2) \\
(20) 4' \ (1/2,0,0) \ x,0,1/2 \\
(2_{yz}) 1/2,1/2,1/2) \\
(24) 2' \ x+1,2/1,4,x \\
(2_{yz}) 1/2,1/2,1/2) \\
(28) n' \ (0,1/2,1/2) \ 1/4,y,z \\
(2_{yz}) 1/2,1/2,1/2) \\
(32) 3' \ x+1,x,x; 3/4,-1/4,1/4 \\
(3_{xyz}) 1/2,1/2,12) \\
(36) 3' \ x+1,x,x; 3/4,1/4,1/4 \\
(3_{xyz}) 1/2,1/2,12) \\

(20) 4' \ (1/2,0,0) \ x,0,1/2 \\
(2_{yz}) 1/2,1/2,1/2) \\
(24) 2' \ x+1,2/1,4,x \\
(2_{yz}) 1/2,1/2,1/2) \\
(28) n' \ (0,1/2,1/2) \ 1/4,y,z \\
(2_{yz}) 1/2,1/2,1/2) \\
(32) 3' \ x+1,x,x; 3/4,-1/4,1/4 \\
(3_{xyz}) 1/2,1/2,12) \\
(36) 3' \ x+1,x,x; 3/4,1/4,1/4 \\
(3_{xyz}) 1/2,1/2,12) \\

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Continued 224.2.1612 Pn\(^3\)m1' 

(37) \( m' \), \( x, x, z \)  
\( (m_{yz}|0,0,0)' \)  
(38) \( m' \), \( x, x, z \)  
\( (m_{xy}|0,0,0)' \)  
(39) \( \bar{4}^{+} \), \( 0,0, z \); \( 0,0,0 \)  
\( (4_{z}^{-}|0,0,0)' \)  
(40) \( \bar{4}^{+} \), \( 0,0, z \); \( 0,0,0 \)  
\( (4_{z}^{-}|0,0,0)' \)  

(41) \( \bar{4}^{-} \), \( x, 0, 0; 0,0,0 \)  
\( (4_{x}^{-}|0,0,0)' \)  
(42) \( m' \), \( x, y, y \)  
\( (m_{yz}|0,0,0)' \)  
(43) \( m' \), \( x, y, y \)  
\( (m_{yz}|0,0,0)' \)  
(44) \( \bar{4}^{-} \), \( 0,0,0 \)  
\( (4_{x}^{-}|0,0,0)' \)  

(45) \( \bar{4}^{-} \), \( 0, y, 0; 0,0,0 \)  
\( (4_{y}^{-}|0,0,0)' \)  
(46) \( m' \), \( x, y, x \)  
\( (m_{x}|0,0,0)' \)  
(47) \( \bar{4}^{-} \), \( 0, y, 0; 0,0,0 \)  
\( (4_{y}^{-}|0,0,0)' \)  
(48) \( m' \), \( x, y, x \)  
\( (m_{x}|0,0,0)' \)  

Generators selected  
(1); \( t(1,0,0); t(0,1,0); t(0,0,1) \); (2); (3); (5); (13); (25); \( 1' \). 

Positions  

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<tr>
<td>1 +</td>
<td>1' +</td>
</tr>
</tbody>
</table>

Continued 224.2.1612 Pn\(^3\)m1' 

48  

(1) \( x, y, z [0,0,0] \)  
(2) \( \bar{x}, \bar{y}, \bar{z} [0,0,0] \)  
(3) \( \bar{x}, \bar{y}, \bar{z} [0,0,0] \)  
(4) \( x, y, z [0,0,0] \)  
(5) \( z, x, y [0,0,0] \)  
(6) \( \bar{z}, \bar{x}, \bar{y} [0,0,0] \)  
(7) \( \overline{z}, x, y [0,0,0] \)  
(8) \( z, x, y [0,0,0] \)  

(9) \( y, z, x [0,0,0] \)  
(10) \( \bar{y}, \bar{z}, \bar{x} [0,0,0] \)  
(11) \( \bar{y}, \bar{z}, \bar{x} [0,0,0] \)  
(12) \( y, z, x [0,0,0] \)  
(13) \( y+1/2, x+1/2, z+1/2 [0,0,0] \)  
(14) \( \bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [0,0,0] \)  
(15) \( y+1/2, x+1/2, z+1/2 [0,0,0] \)  
(16) \( \bar{y}+1/2, \bar{x}+1/2, \bar{z}+1/2 [0,0,0] \)  
(17) \( x+1/2, z+1/2, y+1/2 [0,0,0] \)  
(18) \( \bar{x}+1/2, \bar{z}+1/2, \bar{y}+1/2 [0,0,0] \)  
(19) \( x+1/2, \bar{z}+1/2, \bar{y}+1/2 [0,0,0] \)  
(20) \( \bar{x}+1/2, \bar{z}+1/2, y+1/2 [0,0,0] \)  
(21) \( z+1/2, y+1/2, \bar{x}+1/2 [0,0,0] \)  
(22) \( \bar{z}+1/2, \bar{y}+1/2, x+1/2 [0,0,0] \)  
(23) \( z+1/2, \bar{y}+1/2, \bar{x}+1/2 [0,0,0] \)  
(24) \( \bar{z}+1/2, \bar{y}+1/2, x+1/2 [0,0,0] \)  
(25) \( x+1/2, \bar{y}+1/2, \bar{z}+1/2 [0,0,0] \)  
(26) \( \bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2 [0,0,0] \)  
(27) \( x+1/2, \bar{y}+1/2, \bar{z}+1/2 [0,0,0] \)  
(28) \( \bar{x}+1/2, \bar{y}+1/2, \bar{z}+1/2 [0,0,0] \)  
(29) \( \bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2 [0,0,0] \)  
(30) \( z+1/2, x+1/2, y+1/2 [0,0,0] \)  
(31) \( \bar{z}+1/2, \bar{x}+1/2, \bar{y}+1/2 [0,0,0] \)  
(32) \( z+1/2, \bar{x}+1/2, \bar{y}+1/2 [0,0,0] \)  
(33) \( \bar{y}+1/2, \bar{z}+1/2, x+1/2 [0,0,0] \)  
(34) \( y+1/2, \bar{z}+1/2, x+1/2 [0,0,0] \)  
(35) \( \bar{y}+1/2, \bar{z}+1/2, x+1/2 [0,0,0] \)  
(36) \( y+1/2, \bar{z}+1/2, x+1/2 [0,0,0] \)  

(37) \( \bar{y}, \bar{z}, \overline{z} [0,0,0] \)  
(38) \( y, x, z [0,0,0] \)  
(39) \( \bar{y}, \bar{x}, \bar{z} [0,0,0] \)  
(40) \( y, x, z [0,0,0] \)  
(41) \( x, y, z [0,0,0] \)  
(42) \( x, \bar{z}, \bar{y} [0,0,0] \)  
(43) \( x, \bar{z}, \bar{y} [0,0,0] \)  
(44) \( x, \bar{z}, \bar{y} [0,0,0] \)  

(45) \( z, \bar{y}, \bar{x} [0,0,0] \)  
(46) \( z, \bar{y}, \bar{x} [0,0,0] \)  
(47) \( z, \bar{y}, \bar{x} [0,0,0] \)  
(48) \( z, y, x [0,0,0] \)  

24  

\( x, x, z [0,0,0] \)  
\( \bar{x}, \bar{x}, \bar{z} [0,0,0] \)  
\( \bar{x}, \bar{x}, \bar{z} [0,0,0] \)  
\( x, x, z [0,0,0] \)  
\( z, x, x [0,0,0] \)  
\( \bar{z}, \bar{x}, \bar{x} [0,0,0] \)  
\( \bar{z}, \bar{x}, \bar{x} [0,0,0] \)  
\( x, z, x [0,0,0] \)  
\( \bar{x}, \bar{z}, \bar{x} [0,0,0] \)  
\( \bar{x}, \bar{z}, \bar{x} [0,0,0] \)
Continued

12  f  2.221'  1/4,0,1/2 [0,0,0]  3/4,0,1/2 [0,0,0]  1/2,1/4,0 [0,0,0]
     1/2,3/4,0 [0,0,0]  0,1/2,1/4 [0,0,0]  0,1/2,3/4 [0,0,0]
     1/4,1/2,0 [0,0,0]  3/4,1/2,0 [0,0,0]  0,1/4,1/2 [0,0,0]
     0,3/4,1/2 [0,0,0]  1/2,0,1/4 [0,0,0]  1/2,0,3/4 [0,0,0]

8  e  .3m1'  x,x,x [0,0,0]  x,x,x [0,0,0]
     x,x,x [0,0,0]  x,x,x [0,0,0]
     x+1/2,x+1/2,x+1/2 [0,0,0]  x+1/2,x+1/2,x+1/2 [0,0,0]

6  d  42.m1'  0,1/2,1/2 [0,0,0]  1/2,0,1/2 [0,0,0]  1/2,1/2,0 [0,0,0]
     0,1/2,0 [0,0,0]  1/2,0,0 [0,0,0]  0,0,1/2 [0,0,0]

4  c  3m1'  3/4,3/4,3/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  1/4,3/4,1/4 [0,0,0]
     3/4,3/4,3/4 [0,0,0]  1/4,3/4,1/4 [0,0,0]  3/4,1/4,3/4 [0,0,0]

4  b  3m1'  1/4,1/4,1/4 [0,0,0]  3/4,3/4,1/4 [0,0,0]  3/4,1/4,3/4 [0,0,0]
     1/4,1/4,1/4 [0,0,0]  3/4,3/4,1/4 [0,0,0]  1/4,3/4,3/4 [0,0,0]

2  a  43m1'  0,0,0 [0,0,0]  1/2,1/2,1/2 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]  p4mm1'
\( \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \)
Origin at 0,0,z

Along [1,1,1]  p6mm1'
\( \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \quad \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3 \)
Origin at x,x,x

Along [1,1,0]  2mm1'
\( \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c} \)
Origin at x,x,1/4
Origin at $\overline{4}3m$, at $-1/4,-1/4,-1/4$ from center ($3'm$)

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad y \leq x; \quad \text{max}(x-1/2,-y) \leq z \leq \text{min}(1/2-x,y)$

Vertices

$0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

Symmetry Operations

(1) 1  \hspace{1cm} (2) 2 0,0,z  \hspace{1cm} (3) 2 0,y,0  \hspace{1cm} (4) 2 x,0,0
(1*0,0,0)  (2*0,0,0)  (2*y,0,0)  (2*z,0,0)

(5) $3^+ x,x,x$  \hspace{1cm} (6) $3^+ x,x,x$  \hspace{1cm} (7) $3^+ x,x,x$  \hspace{1cm} (8) $3^+ x,x,x$
($3_{xyz}[0,0,0]$  ($3_{xyz}[0,0,0]$  ($3_{xyz}[0,0,0]$  ($3_{xyz}[0,0,0]$)

(9) $3^- x,x,x$  \hspace{1cm} (10) $3^- x,x,x$  \hspace{1cm} (11) $3^- x,x,x$  \hspace{1cm} (12) $3^- x,x,x$
($3_{xyz}^{-1}[0,0,0]$  ($3_{xyz}^{-1}[0,0,0]$  ($3_{xyz}^{-1}[0,0,0]$  ($3_{xyz}^{-1}[0,0,0]$)

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Continued

**Positions**

<table>
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<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
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1. $x, y, z$ [u,v,w]
2. $\bar{x}, \bar{y}, \bar{z}$ [u,\bar{v},w]
3. $\bar{x}, y, \bar{z}$ [\bar{u},v,w]
4. $x, \bar{y}, \bar{z}$ [u,\bar{v},w]

5. $z, x, y$ [w,u,v]
6. $\bar{z}, x, \bar{y}$ [w,\bar{u},v]
7. $\bar{z}, \bar{x}, y$ [w,\bar{u},v]
8. $\bar{z}, x, y$ [w,u,\bar{v}]

9. $y, z, x$ [v,w,u]
10. $y, z, x$ [v,w,u]
11. $\bar{y}, z, \bar{x}$ [v,\bar{w},u]
12. $\bar{y}, z, x$ [v,\bar{w},u]

(13) $y+1/2, x+1/2, \bar{z}+1/2 [v, u, w]$ (14) $y+1/2, x+1/2, z+1/2 [v, u, w]$ (15) $y+1/2, x+1/2, z+1/2 [v, u, \bar{w}]$ (16) $y+1/2, x+1/2, z+1/2 [v, \bar{u}, w]$

(17) $x+1/2, z+1/2, \bar{y}+1/2 [u, w, v]$ (18) $x+1/2, z+1/2, y+1/2 [u, w, v]$ (19) $x+1/2, \bar{z}+1/2, y+1/2 [u, w, \bar{v}]$ (20) $x+1/2, \bar{z}+1/2, y+1/2 [u, \bar{w}, v]$

(21) $z+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$ (22) $z+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$ (23) $\bar{z}+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$ (24) $\bar{z}+1/2, y+1/2, x+1/2 [\bar{w}, v, u]$

(25) $\bar{z}+1/2, \bar{z}+1/2, z+1/2 [u, \bar{v}, w]$ (26) $\bar{z}+1/2, \bar{z}+1/2, \bar{z}+1/2 [u, \bar{v}, w]$ (27) $\bar{z}+1/2, y+1/2, z+1/2 [u, \bar{v}, w]$ (28) $\bar{z}+1/2, y+1/2, \bar{z}+1/2 [u, \bar{v}, w]$

(29) $\bar{z}+1/2, \bar{z}+1/2, \bar{z}+1/2 [\bar{u}, \bar{v}, w]$ (30) $\bar{z}+1/2, \bar{z}+1/2, \bar{z}+1/2 [\bar{u}, \bar{v}, w]$ (31) $\bar{z}+1/2, \bar{z}+1/2, \bar{z}+1/2 [\bar{u}, \bar{v}, w]$ (32) $\bar{z}+1/2, \bar{z}+1/2, \bar{z}+1/2 [\bar{u}, \bar{v}, w]$

(33) $\bar{y}+1/2, \bar{z}+1/2, x+1/2 [v, w, u]$ (34) $\bar{y}+1/2, \bar{z}+1/2, x+1/2 [v, w, u]$ (35) $\bar{y}+1/2, \bar{z}+1/2, x+1/2 [v, w, u]$ (36) $\bar{y}+1/2, \bar{z}+1/2, x+1/2 [v, w, u]$
Symmetry of Special Projections

Along \([0,0,1]\) \(p4\'mm'\)

- \(a^* = (a - b)/2\)
- \(b^* = (a + b)/2\)

Origin at \(0,0,z\)

Along \([1,1,1]\) \(p6mm\)

- \(a^* = (2a - b - c)/3\)
- \(b^* = (-a + 2b - c)/3\)

Origin at \(x,x,x\)

Along \([1,1,0]\) \(p2mm1'\)

- \(a^* = (-a + b)/2\)
- \(b^* = c\)

Origin at \(x,x,1/4\)
Origin at $\overline{4}3m'$, at $-1/4,-1/4,-1/4$ from center ($\overline{3}m'$)

Asymmetric unit  

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad y \leq x; \quad \max(x-1/2,-y) \leq z \leq \min(1/2-x,y)$

Vertices  

$0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4$

Symmetry Operations

1. $1$
2. $2 \begin{pmatrix} 0,0,z \end{pmatrix}$
3. $2 \begin{pmatrix} 0,y,0 \end{pmatrix}$
4. $2 \begin{pmatrix} x,0,0 \end{pmatrix}$

5. $3^+ \begin{pmatrix} x,x,x \end{pmatrix}$
6. $3^+ \begin{pmatrix} x,x,x \end{pmatrix}$
7. $3^+ \begin{pmatrix} x,x,x \end{pmatrix}$
8. $3^- \begin{pmatrix} x,x,x \end{pmatrix}$

9. $3^- \begin{pmatrix} 0,0,0 \end{pmatrix}$
10. $3^- \begin{pmatrix} 0,0,0 \end{pmatrix}$
11. $3^- \begin{pmatrix} 0,0,0 \end{pmatrix}$
12. $3^- \begin{pmatrix} 0,0,0 \end{pmatrix}$
Continued 224.2.1612 Pn\( \bar{3} \)m1'

| (13) 2' (1/2,1/2,0) | (x,x,1/4) (2_{xy}|1/2,1/2,1/2)' |
| (14) 2' | (x,x+1/2,1/4) (2_{xy}|1/2,1/2,1/2)' |
| (15) 4' | (0,0,1/2) | (2_{xy}|1/2,1/2,1/2)' |
| (16) 4' | (0,0,1/2) | (2_{xy}|1/2,1/2,1/2)' |

| (17) 4' | (1/2,0,0) | (x,1/2,0) (4_{x}|1/2,1/2,1/2)' |
| (18) 2' | (0,1/2,1/2) | (1/4,y,y) (2_{xy}|1/2,1/2,1/2)' |
| (19) 2' | (1/4,y+1/2,y) (2_{xy}|1/2,1/2,1/2)' |
| (20) 4'' | (1/2,0,0) | (x,0,1/2) (4_{x}|1/2,1/2,1/2)' |

| (21) 4'' | (0,1/2,0) | (1/2,y,0) (4_{y}|1/2,1/2,1/2)' |
| (22) 2' | (1/2,0,1/2) | (x,1/4,x) (2_{xy}|1/2,1/2,1/2)' |
| (23) 4'' | (0,1/2,0) | (0,y,1/2) (4_{x}|1/2,1/2,1/2)' |
| (24) 2' | (x+1/2,1/4,x) (2_{xy}|1/2,1/2,1/2)' |

| (25) | 1/4,1,4,1/4 | (1/2,1/2,1,12) |
| (26) n | (1/2,1/2,0) | (x,y,1/4) (m_{xy}|1/2,1/2,12) |
| (27) n | (1/2,0,1/2) | (x,1/4,z) (m_{xy}|1/2,1/2,12) |
| (28) n | (0,1/2,1/2) | (1/4,y,z) (m_{xy}|1/2,1/2,12) |

| (29) 3' | x,x,x; | 1/4,1,4,1/4 |
| (30) 3' | x-1,x+1,-x; | 1/4,1,4,3/4 |
| (31) 3' | x+1,x; | 1/4,3/4,-1/4 |
| (32) 3' | x+1,x; | 3/4,-1/4,1/4 |

| (33) 3' | x,x,x; | 1/4,1,4,1/4 |
| (34) 3' | x+1,-x-1,x; | 1/4,-1/4,3/4 |
| (35) 3' | x,x+1,-x; | -1/4,3/4,1/4 |
| (36) 3' | x+1,x; | 3/4,1/4,-1/4 |

| (37) m' | x,x,z | (m_{yz}|0,0,0)' |
| (38) m' | x,x,z | (m_{yz}|0,0,0)' |
| (39) 4'' | 0,0,z; | 0,0,0 |
| (40) 4'' | 0,0,z; | 0,0,0 |

| (41) 4'' | x,0,0; | 0,0,0 |
| (42) m' | x,y,y | (m_{yz}|0,0,0)' |
| (43) m' | x,y,y | (m_{yz}|0,0,0)' |
| (44) 4'' | x,0,0; | 0,0,0 |
| (45) 4'' | y,0,0; | 0,0,0 |
| (46) m' | x,y,x | (m_{yz}|0,0,0)' |
| (47) 4'' | y,0,0; | 0,0,0 |
| (48) m' | x,y,x | (m_{yz}|0,0,0)' |

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48 1 1

| (1) x,y,z | [u,v,w] |
| (2) x,y,z | [u,v,w] |
| (3) x,y,z | [u,v,w] |
| (4) x,y,z | [u,v,w] |

| (5) x,z,y | [w,u,v] |
| (6) z,x,y | [w,u,v] |
| (7) z,x,y | [w,u,v] |
| (8) z,x,y | [w,u,v] |

| (9) y,z,x | [v,w,u] |
| (10) y,z,x | [v,w,u] |
| (11) y,z,x | [v,w,u] |
| (12) y,z,x | [v,w,u] |

| (13) y+1/2,x+1/2,z+1/2 | [v,u,w] |
| (14) y+1/2,x+1/2,z+1/2 | [v,u,w] |
| (15) y+1/2,x+1/2,z+1/2 | [v,u,w] |
| (16) y+1/2,x+1/2,z+1/2 | [v,u,w] |

| (17) x+1/2,z+1/2,y+1/2 | [u,w,v] |
| (18) x+1/2,z+1/2,y+1/2 | [u,w,v] |
| (19) x+1/2,z+1/2,y+1/2 | [u,w,v] |
| (20) x+1/2,z+1/2,y+1/2 | [u,w,v] |

| (21) z+1/2,y+1/2,x+1/2 | [w,v,u] |
| (22) z+1/2,y+1/2,x+1/2 | [w,v,u] |
| (23) z+1/2,y+1/2,x+1/2 | [w,v,u] |
| (24) z+1/2,y+1/2,x+1/2 | [w,v,u] |

| (25) z+1/2,y+1/2,z+1/2 | [w,u,v] |
| (26) x+1/2,y+1/2,z+1/2 | [u,v,w] |
| (27) x+1/2,y+1/2,z+1/2 | [u,v,w] |
| (28) x+1/2,y+1/2,z+1/2 | [u,v,w] |

| (29) z+1/2,x+1/2,y+1/2 | [w,u,v] |
| (30) z+1/2,x+1/2,y+1/2 | [w,u,v] |
| (31) z+1/2,x+1/2,y+1/2 | [w,u,v] |
| (32) z+1/2,x+1/2,y+1/2 | [w,u,v] |

| (33) y+1/2,z+1/2,x+1/2 | [v,w,u] |
| (34) y+1/2,z+1/2,x+1/2 | [v,w,u] |
| (35) y+1/2,z+1/2,x+1/2 | [v,w,u] |
| (36) y+1/2,z+1/2,x+1/2 | [v,w,u] |

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<th>Continued</th>
<th>224.2.1612</th>
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\[\begin{align*}
\bar{x} + 1/2, 1/2, 0 & \quad [u, 0, 0] & \bar{x} + 1/2, 1/2, 0 & \quad [\bar{u}, 0, 0] & 0, x + 1/2, 1/2 & \quad [0, u, 0] & 0, x + 1/2, 1/2 & \quad [0, \bar{u}, 0] \\
1/2, 0, x + 1/2 & \quad [0, 0, u] & 1/2, 0, x + 1/2 & \quad [0, 0, \bar{u}] & 0, x + 1/2 & \quad [0, u, 0] & 0, x + 1/2 & \quad [0, \bar{u}, 0] \\
\bar{x}, 1/2, 0 & \quad [\bar{u}, 0, 0] & x, 1/2 & \quad [u, 0, 0] & 1/2, 0, x & \quad [0, 0, u] & 1/2, 0, x & \quad [0, 0, \bar{u}] \\
\end{align*}\]

12 \quad g \quad 2m'm' \quad x, 0, 0 & \quad [u, 0, 0] & \bar{x}, 0, 0 & \quad [\bar{u}, 0, 0] & 0, x & \quad [0, u, 0] & 0, \bar{x}, 0 & \quad [0, \bar{u}, 0] \\
0, 0, x & \quad [0, 0, u] & 0, 0, x & \quad [0, u, 0] & 1/2, x + 1/2, 1/2 & \quad [0, u, 0] & 1/2, x + 1/2, 1/2 & \quad [0, \bar{u}, 0] \\
x + 1/2, 1/2, 1/2 & \quad [u, 0, 0] & \bar{x} + 1/2, 1/2, 1/2 & \quad [\bar{u}, 0, 0] & 1/2, 1/2, x + 1/2 & \quad [0, u, 0] & 1/2, 1/2, x + 1/2 & \quad [0, \bar{u}, 0] \\
\end{align*}\]

12 \quad f \quad 222' \quad 1/4, 0, 1/2 & \quad [u, 0, 0] & 3/4, 0, 1/2 & \quad [\bar{u}, 0, 0] & 1/2, 1/4, 0 & \quad [0, u, 0] \\
1/2, 3/4, 0 & \quad [0, \bar{u}, 0] & 0, 1/2, 1/4 & \quad [0, 0, u] & 0, 1/2, 3/4 & \quad [0, 0, \bar{u}] \\
1/4, 1/2, 0 & \quad [u, 0, 0] & 3/4, 1/2, 0 & \quad [\bar{u}, 0, 0] & 0, 1/4, 1/2 & \quad [0, u, 0] \\
0, 3/4, 1/2 & \quad [0, \bar{u}, 0] & 1/2, 0, 1/4 & \quad [0, 0, u] & 1/2, 0, 3/4 & \quad [0, 0, \bar{u}] \\
\end{align*}\]

8 \quad e \quad .3m' \quad x, x, x & \quad [u, u, u] & \bar{x}, x, x & \quad [\bar{u}, u, u] \\
x, x, x & \quad [u, u, \bar{u}] & x, x, x & \quad [u, u, u] \\
x + 1/2, x + 1/2, x + 1/2 & \quad [\bar{u}, \bar{u}, u] & \bar{x} + 1/2, x + 1/2, x + 1/2 & \quad [u, u, u] \\
x + 1/2, x + 1/2, x + 1/2 & \quad [\bar{u}, \bar{u}, u] & \bar{x} + 1/2, x + 1/2, x + 1/2 & \quad [u, u, u] \\
\end{align*}\]

6 \quad d \quad 4'2m' \quad 0, 1/2, 1/2 & \quad [0, 0, 0] & 1/2, 0, 1/2 & \quad [0, 0, 0] & 1/2, 1/2, 0 & \quad [0, 0, 0] \\
0, 1/2, 0 & \quad [0, 0, u] & 1/2, 0, 0 & \quad [0, 0, 0] & 0, 0, 1/2 & \quad [0, 0, 0] \\
\end{align*}\]

4 \quad c \quad .3m' \quad 3/4, 3/4, 1/4 & \quad [u, u, u] & 1/4, 1/4, 3/4 & \quad [\bar{u}, \bar{u}, u] & 1/4, 1/4, 1/4 & \quad [u, u, u] & 3/4, 1/4, 1/4 & \quad [\bar{u}, \bar{u}, u] \\
4 \quad b \quad .3m' \quad 1/4, 1/4, 1/4 & \quad [u, u, u] & 3/4, 3/4, 1/4 & \quad [\bar{u}, \bar{u}, u] & 3/4, 1/4, 3/4 & \quad [u, u, u] & 1/4, 3/4, 3/4 & \quad [\bar{u}, \bar{u}, u] \\
2 \quad a \quad 4'3m' \quad 0, 0, 0 & \quad [0, 0, 0] & 1/2, 1/2, 1/2 & \quad [0, 0, 0] \\
\end{align*}\]

Symmetry of Special Projections

Along [0, 0, 1] \quad p4mm1' \quad \begin{align*}
a^* &= (a - b)/2 & b^* &= (a + b)/2 \\
\text{Origin at } 0, 0, z \\
\end{align*}
Along [1, 1, 1] \quad p6'mm' \quad \begin{align*}
a^* &= (2a - b - c)/3 & b^* &= (-a + 2b - c)/3 \\
\text{Origin at } x, x, x \\
\end{align*}
Along [1, 1, 0] \quad p2'mm' \quad \begin{align*}
a^* &= a & b^* &= -(a + b)/2 \\
\text{Origin at } x, x, 1/4 \\
\end{align*}
Origin at $4\bar{3}m'$, at $-1/4,-1/4,-1/4$ from center ($\bar{3}m'$)

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad -1/4 \leq z \leq 1/4; \quad y \leq x; \quad \max(x-1/2,-y) \leq z \leq \min(1/2-x,y)\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4 \quad 1/4,1/4,-1/4\]

Symmetry Operations

1. \[1\]
2. \[2, 0,0,z\]
3. \[2, 0,y,0\]
4. \[2, x,0,0\]
5. \[3 \cdot x,x,x\]
6. \[3 \cdot x,x,x\]
7. \[3 \cdot x,x,x\]
8. \[3 \cdot x,x,x\]
9. \[3 \cdot x,x,x\]
10. \[3 \cdot x,x,x\]
11. \[3 \cdot x,x,x\]
12. \[3 \cdot x,x,x\]
Continued

\[\begin{array}{llll}
(13) & 2 (1/2,1/2,0) & x,x,1/4 & (14) & 2 \ x,x+1/2,1/4 \\
      & (2_{xy}) & 1/2,1/2,1/2 & (2_{xy}) & 1/2,1/2,1/2 \\
(17) & 4 (1/2,0,0) & x,1/2,0 & (18) & 2 (0,1/2,1/2) & 1/4,y,y \\
      & (4_{-x}^{-1}) & 1/2,1/2,1/2 & (2_{yz}) & 1/2,1/2,1/2 \\
(21) & 4 (0,1/2,0) & 1/2,y,0 & (22) & 2 (1/2,1/2,1/2) & x,1/4,x \\
      & (4_{y}) & 1/2,1/2,1/2 & (2_{xz}) & 1/2,1/2,1/2 \\
(25) & \tilde{1} & 1/4,1/4,1/4 & (26) & n' (1/2,1/2,0) & x,y,1/4 \\
      & (1,1/2,1/2,12)' & & (27) & n' (1/2,1/2,1/2)' & x,1/4,z \\
(29) & \tilde{3}^{-+} & x,x,x; 1/4,1/4,1/4 & (30) & \tilde{3}^{-+} & x,x+1,1,x; -1/4,1/4,3/4 \\
      & (3_{xyz}) & 1/2,1/2,12)' & (3_{xyz}) & 1/2,1/2,12)' & 1/4,3/4,1/4 \\
(33) & \tilde{3}^{-+} & x,x,x; 1/4,1/4,1/4 & (34) & \tilde{3}^{-+} & x,x+1,1,x; -1/4,3/4,1/4 \\
      & (3_{xyz}) & 1/2,1/2,12)' & (3_{xyz}) & 1/2,1/2,12)' & 3/4,1/4,-1/4 \\
(37) & m' & x,x,z & (38) & m' & x,y,0 \\
      & (m_{xy}) & 0,0,0)' & & (m_{xy}) & 0,0,0)' \\
(41) & \tilde{4}^{-+} & x,0,0; 0,0,0 & (42) & m' & x,y,y \\
      & (4_{-z}^{-1}) & 0,0,0)' & & (m_{yz}) & 0,0,0)' \\
(45) & \tilde{4}^{-+} & y,0,0; 0,0,0 & (46) & m' & x,x,x \\
      & (4_{z}^{-1}) & 0,0,0)' & & (m_{xz}) & 0,0,0)' \\
\end{array}\]

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

48  1

<table>
<thead>
<tr>
<th>1</th>
<th>1</th>
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</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x, y, z [u, v, w]</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(6) z, x, y [w, u, v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) y, z, x [v,w,u]</td>
</tr>
<tr>
<td>(13) y+1/2, x+1/2, z+1/2 [v,w,u]</td>
<td>(14) y+1/2, x+1/2, z+1/2 [v,w,u]</td>
</tr>
<tr>
<td>(17) x+1/2, z+1/2, y+1/2 [u,w,v]</td>
<td>(18) x+1/2, z+1/2, y+1/2 [u,w,v]</td>
</tr>
<tr>
<td>(21) z+1/2, y+1/2, x+1/2 [w,v,u]</td>
<td>(22) z+1/2, y+1/2, x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(25) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
<td>(26) x+1/2, y+1/2, z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(29) z+1/2, x+1/2, y+1/2 [w,u,v]</td>
<td>(30) z+1/2, x+1/2, y+1/2 [w,u,v]</td>
</tr>
<tr>
<td>(33) y+1/2, z+1/2, x+1/2 [v,w,u]</td>
<td>(34) y+1/2, z+1/2, x+1/2 [v,w,u]</td>
</tr>
</tbody>
</table>

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5); (13); (25).

Coordinates
Continued

<table>
<thead>
<tr>
<th>224.5.1615</th>
<th>Pn'3'm'</th>
</tr>
</thead>
</table>

| (37) $\bar{y}, x, z [v, u, w]$ | (38) $y, x, z [v, u, w]$ | (39) $\bar{y}, x, z [v, u, w]$ | (40) $y, x, z [v, u, w]$ |
| (41) $x, z, y [u, w, v]$ | (42) $x, z, y [u, w, v]$ | (43) $x, z, y [u, w, v]$ | (44) $x, z, y [u, w, v]$ |
| (45) $\bar{z}, y, x [w, v, u]$ | (46) $\bar{z}, y, x [w, v, u]$ | (47) $\bar{z}, y, x [w, v, u]$ | (48) $z, y, x [w, v, u]$ |

24 \quad k \quad \ldots m'

\begin{align*}
x, x, z [u, u, w] & \quad \bar{x}, x, z [u, u, w] \\
z, x, x [w, u, u] & \quad \bar{z}, x, x [w, u, u] \\
x, z, x [u, u, w] & \quad \bar{x}, z, x [u, u, w] \\
x + 1/2, x + 1/2, z + 1/2 [u, u, w] & \quad \bar{x} + 1/2, x + 1/2, z + 1/2 [u, u, w] \\
x + 1/2, z + 1/2, x + 1/2 [u, w, u] & \quad \bar{x} + 1/2, z + 1/2, x + 1/2 [u, w, u] \\
z + 1/2, x + 1/2, x + 1/2 [w, u, u] & \quad \bar{z} + 1/2, x + 1/2, x + 1/2 [w, u, u] \\
\end{align*}

24 \quad j \quad \ldots 2

\begin{align*}
1/4, y, y + 1/2 [0, v, v] & \quad 3/4, \bar{y}, y + 1/2 [0, v, v] \\
y + 1/2, 1/4, y [v, 0, v] & \quad y + 1/2, 3/4, y [v, 0, v] \\
y, y + 1/2, 1/4 [v, v, 0] & \quad \bar{y}, \bar{y} + 1/2, 3/4 [v, v, 0] \\
1/4, \bar{y} + 1/2, \bar{y} [0, v, v] & \quad 3/4, y + 1/2, y [0, v, v] \\
\bar{y}, 1/4, \bar{y} + 1/2 [v, 0, v] & \quad y, 3/4, \bar{y} + 1/2 [v, 0, v] \\
\bar{y} + 1/2, y, 1/4 [v, v, 0] & \quad y + 1/2, \bar{y}, 3/4 [v, v, 0] \\
\end{align*}

24 \quad i \quad \ldots 2

\begin{align*}
1/4, y, \bar{y} + 1/2 [0, v, v] & \quad 3/4, y, \bar{y} + 1/2 [0, v, v] \\
y + 1/2, 1/4, y [v, 0, v] & \quad y + 1/2, 3/4, y [v, 0, v] \\
y, \bar{y} + 1/2, 1/4 [v, v, 0] & \quad \bar{y}, y + 1/2, 3/4 [v, v, 0] \\
1/4, \bar{y}, \bar{y} + 1/2, \bar{y} [0, v, v] & \quad 3/4, y + 1/2, y [0, v, v] \\
y, 1/4, \bar{y} + 1/2 [v, 0, v] & \quad y, 3/4, \bar{y} + 1/2 [v, 0, v] \\
\bar{y} + 1/2, y, 1/4 [v, v, 0] & \quad y + 1/2, \bar{y}, 3/4 [v, v, 0] \\
\end{align*}

24 \quad h \quad \ldots 2

\begin{align*}
x, 0, 1/2 [u, 0, 0] & \quad \bar{x}, 0, 1/2 [u, 0, 0] \\
0, 1/2, x [0, 0, u] & \quad 0, 1/2, \bar{x} [0, 0, \bar{u}] \\
x + 1/2, 0, 1/2 [u, 0, 0] & \quad x + 1/2, 0, 1/2 [u, 0, 0] \\
\end{align*}

224.5.1615 - 3 - 3711
Continued

### Symmetry of Special Projections

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<tr>
<th>12</th>
<th>g</th>
<th>2.m'm'</th>
<th>x,0,0 [u,0,0]</th>
<th>x,0,0 [u,0,0]</th>
<th>0,x,0 [0,u,0]</th>
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<td>1/2,0,x+1/2 [0,u,0]</td>
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<th>8</th>
<th>e</th>
<th>.3m'</th>
<th>x,x,x [u,u,u]</th>
<th>x,x,x [u,u,u]</th>
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<tr>
<td>0,0,x [0,0,u]</td>
<td>0,0,x [0,0,u]</td>
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<th>1/2,0,1/2 [0,0,0]</th>
<th>1/2,1/2,0 [0,0,0]</th>
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<td>1/2,0,0 [0,0,0]</td>
<td>0,0,1/2 [0,0,0]</td>
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<th>1/4,1,4,3/4 [0,0,0]</th>
<th>1/4,3,1/4,4 [0,0,0]</th>
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<td>3/4,3,1/4,4 [0,0,0]</td>
<td>1/4,3,1/4,4 [0,0,0]</td>
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<td>1/2,x+1/2,x+1/2 [0,0,u]</td>
<td>1/2,x+1/2,x+1/2 [0,0,u]</td>
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### Origin at 0,0,z

\( \mathbf{a}^* = \frac{\mathbf{a} - \mathbf{b}}{2} \)
\( \mathbf{b}^* = \frac{\mathbf{a} + \mathbf{b}}{2} \)

### Origin at x,x,x

\( \mathbf{a}^* = \frac{(2\mathbf{a} - \mathbf{b} - \mathbf{c})}{3} \)
\( \mathbf{b}^* = \frac{(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})}{3} \)

### Origin at x,x,1/4

\( \mathbf{a}^* = \frac{(-\mathbf{a} + \mathbf{b})}{2} \)
\( \mathbf{b}^* = \mathbf{c} \)
**Origin** at $\bar{4}3m$, at $-1/4,-1/4,-1/4$ from center ($\bar{3}m$)

**Asymmetric unit**

\[
\begin{align*}
0 \leq x & \leq 1/2; \\
0 \leq y & \leq 1/2; \\
-1/4 \leq z & \leq 1/4; \\
y & \leq x; \\
\max(x-1/2,-y) & \leq z \leq \min(1/2-x,y)
\end{align*}
\]

**Symmetry Operations**

<table>
<thead>
<tr>
<th>Set</th>
<th>Operation</th>
<th>Description</th>
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<tbody>
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<td>(1)</td>
<td>1</td>
<td>$m_{x,y,z}$ 0,0,0</td>
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<tr>
<td></td>
<td>(1) 0,0,0</td>
<td>$m_{x,y,z}$ 0,0,0</td>
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<td></td>
<td>(1) 0,0,0</td>
<td>$m_{x,y,z}$ 0,0,0</td>
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<tr>
<td>(5)</td>
<td>$3^* x,x,x$</td>
<td>$(3_{xyz})^* 0,0,0$</td>
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<td>$(3_{xyz})^* 0,0,0$</td>
<td>$(3_{xyz})^* 0,0,0$</td>
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<td>(9)</td>
<td>$3^* x,x,x$</td>
<td>$(3_{xyz})^* 0,0,0$</td>
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<td>$(3_{xyz})^* 0,0,0$</td>
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<td>$2 (1/2,1/2,0)$</td>
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<td>(17)</td>
<td>$4^* (1/2,0,0)$</td>
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<tr>
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<td>(21)</td>
<td>$4^* (1/2,0,0)$</td>
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<tr>
<td>(25)</td>
<td>$\bar{1} 1/4,1/4,1/4$</td>
<td>$n_{x,y,z}$ 0,0,0</td>
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<tr>
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<td>$(1_{xy})^* 1/2,1/2,1/2$</td>
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<tr>
<td>(29)</td>
<td>$3^* x,x,x$</td>
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<td>(33)</td>
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<tr>
<td>(37)</td>
<td>$m x,y,z$</td>
<td>$(m_{x,y,z}) 0,0,0$</td>
</tr>
<tr>
<td></td>
<td>$(m_{x,y,z}) 0,0,0$</td>
<td>$(m_{x,y,z}) 0,0,0$</td>
</tr>
<tr>
<td></td>
<td>$(m_{x,y,z}) 0,0,0$</td>
<td>$(m_{x,y,z}) 0,0,0$</td>
</tr>
<tr>
<td>(41)</td>
<td>$4^* x,0,0$</td>
<td>$(4_{y})^* 0,0,0$</td>
</tr>
<tr>
<td></td>
<td>$(4_{y})^* 0,0,0$</td>
<td>$(4_{y})^* 0,0,0$</td>
</tr>
<tr>
<td>(45)</td>
<td>$4^* y,0,0$</td>
<td>$(4_{y})^* 0,0,0$</td>
</tr>
<tr>
<td></td>
<td>$(4_{y})^* 0,0,0$</td>
<td>$(4_{y})^* 0,0,0$</td>
</tr>
</tbody>
</table>

**For (0,0,0) + set**

<table>
<thead>
<tr>
<th>Set</th>
<th>Operation</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>(1)</td>
<td>$t^* (1,0,0)$</td>
<td>$m_{x,y,z}$ 0,0,0</td>
</tr>
<tr>
<td></td>
<td>(1) 1,0,0</td>
<td>$(m_{x,y,z}) 0,0,0$</td>
</tr>
<tr>
<td>(5)</td>
<td>$3^* (1,3,1/3,3/1)$</td>
<td>$(3_{xyz})^* 1/2,1/2,1/2$</td>
</tr>
<tr>
<td></td>
<td>$(3_{xyz})^* 1/2,1/2,1/2$</td>
<td>$(3_{xyz})^* 1/2,1/2,1/2$</td>
</tr>
<tr>
<td>(9)</td>
<td>$3^* (1,3,1/3,3/1)$</td>
<td>$(3_{xyz})^* 1/2,1/2,1/2$</td>
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<td>$(3_{xyz})^* 1/2,1/2,1/2$</td>
<td>$(3_{xyz})^* 1/2,1/2,1/2$</td>
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</tbody>
</table>
Continued 224.6.1616 Pn3m

(13) 2' x+1/2, x, 1/4
(24) 2' (1/2, 1/2, 0) x, x - 1/2, 1/4
(25) 2' x, y - 1/2, x - 1/4
(36) 2' (1/2, 0, 1/2) x + 1/2, y - 1/2, 1/4

Generators selected 1; t'(1,0,0); t'(0,1,0); t'(0,0,1); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
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<tbody>
<tr>
<td>(1,0,0)</td>
<td>(0,0,0) + (1,0,0)' +</td>
</tr>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(2) x,y,z [u,v,w]</td>
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<td>(5) z,x,y [w,u,v]</td>
<td>(6) z,x,y [w,u,v]</td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td>(10) y,z,x [v,w,u]</td>
</tr>
<tr>
<td>(13) y+1/2, x+1/2, z+1/2 [v,u,w]</td>
<td>(14) y+1/2, x+1/2, z+1/2 [v,u,w]</td>
</tr>
<tr>
<td>(17) x+1/2, z+1/2, y+1/2 [u,w,v]</td>
<td>(18) x+1/2, z+1/2, y+1/2 [u,w,v]</td>
</tr>
<tr>
<td>(21) z+1/2, y+1/2, x+1/2 [w,v,u]</td>
<td>(22) z+1/2, y+1/2, x+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(25) x+1/2, y+1/2, z+1/2 [w,v,u]</td>
<td>(26) x+1/2, y+1/2, z+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(29) z+1/2, y+1/2, x+1/2 [w,v,u]</td>
<td>(30) z+1/2, x+1/2, y+1/2 [w,v,u]</td>
</tr>
<tr>
<td>(33) y+1/2, z+1/2, x+1/2 [v,w,u]</td>
<td>(34) y+1/2, z+1/2, x+1/2 [v,w,u]</td>
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224.6.1616 - 3 - 3715
Continued

<table>
<thead>
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<th>224.6.1616 P F n3m</th>
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</thead>
</table>

\[
x + 1/2, 1/2, 0 [0, v, w] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x + 1/2, 1/2, 0 [0, v, w] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x + 1/2, 1/2, 0 [0, v, w] + 1/2, 1/2, 0 [0, v, w]
\]

<table>
<thead>
<tr>
<th>24 g 2.mm</th>
<th>24 f 2'2'2</th>
</tr>
</thead>
</table>

\[
x, 0, 0 [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, 0, 0 [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, 0, 0 [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

<table>
<thead>
<tr>
<th>16 e .3m</th>
<th>12 d 4'2'm</th>
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</table>

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

<table>
<thead>
<tr>
<th>8 c .3'm</th>
<th>8 b .3'm</th>
</tr>
</thead>
</table>

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

<table>
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<th>4 a 4'3m</th>
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</thead>
</table>

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

\[
x, x, x [0, 0, 0] + 1/2, 1/2, 0 [0, v, w]
\]

**Symmetry of Special Projections**

- **Along [0,0,1]** $p4mm1'$
  \[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \]
  \[ \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2 \]
  \( \text{Origin at } 0,0,z \)

- **Along [1,1,1]** $p6mm1$
  \[ \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \]
  \[ \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3 \]
  \( \text{Origin at } x,x,x \)

- **Along [1,1,0]** $p2mm1$
  \[ \mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \]
  \[ \mathbf{b}^* = \mathbf{c} \]
  \( \text{Origin at } x,x,1/4 \)
Origin at $\bar{4}3m'$, at -1/4,-1/4,-1/4 from center ($\bar{3}m'$)

Asymmetric unit

$0 \leq x \leq 1/2;$ $0 \leq y \leq 1/2;$ $-1/4 \leq z \leq 1/4;$

$y \leq x$; max$(x-1/2,-y) \leq z \leq \min(1/2-x,y)$

Vertices

$0,0,0$ $1/2,0,0$ $1/2,1/2,0$ $1/4,1/4,1/4$ $1/4,1/4,-1/4$

Symmetry Operations

For $(0,0,0)$ + set

(1) 1

(1 0,0,0)

(2) 2' $0,0,z$

(2z | 0,0,0)

(3) 2' $0,y,0$

(2y | 0,0,0)

(4) 2' $x,0,0$

(2x | 0,0,0)

(5) $3^* x,x,x$

($3_{xyz}$ | 0,0,0)

(6) $3^* x,y,x$

($3_{xyz}^{-1}$ | 0,0,0)

(7) $3^* x,x,y$

($3_{xyz}^{-1}$ | 0,0,0)

(8) $3^* x,x,x$

($3_{xyz}$ | 0,0,0)

(9) $3^* x,x,x$

($3_{xyz}^{-1}$ | 0,0,0)

(10) $3^* x,x,x$

($3_{xyz}$ | 0,0,0)

(11) $3^* x,x,x$

($3_{xyz}$ | 0,0,0)

(12) $3^* x,x,x$

($3_{xyz}$ | 0,0,0)

(13) $2' (1/2,1/2,0)$ $x,x,1/4$

($2x | 1/2,1/2,1/2$)

(14) $2' x,x,1+1/2,1/4$

($2x | 1/2,1/2,1/2$)

(15) $4^* (0,0,1/2) 1/2,0,z$

($4z | 1/2,1/2,1/2$)

(16) $4^* (0,0,1/2) 0,1/2,z$

($4z | 1/2,1/2,1/2$)

(17) $4^* (1/2,0,0) x,1/2,0$

($4x | 1/2,1/2,1/2$)

(18) $2' (0,1/2,1/2) y,1/4,y$

($2y | 1/2,1/2,1/2$)

(19) $2' 1/4,y+1/2,y$

($2y | 1/2,1/2,1/2$)

(20) $4^* (1/2,0,0) x,0,1/2$

($4x | 1/2,1/2,1/2$)

(21) $4^* (0,1/2,0) 1/2,y,0$

($4y | 1/2,1/2,1/2$)

(22) $2' (1/2,1/2,0) x,1/4,x$

($2z | 1/2,1/2,1/2$)

(23) $3^* (0,1/2,0) 0,y,1/2$

($3x | 1/2,1/2,1/2$)

(24) $2' 1+1/2,1/4,x$

($2x | 1/2,1/2,1/2$)

(25) $3^* 1/4,1/4,1/4$

($1 | 1/2,1/2,1/2$)

(26) $n (1/2,1/2,0) x,y,1/4$

($m | 1/2,1/2,1/2$)

(27) $m (1/2,0,1/2) x,1/4,z$

($m | 1/2,1/2,1/2$)

(28) $n (0,1/2,1/2) 1/4,y,z$

($m | 1/2,1/2,1/2$)

(29) $3^* x,x,x; 1/4,1/4,1/4$

($3 | 1/2,1/2,1/2$)

(30) $3^* x,-1+x,1+x; -1/4,1/4,3/4$

($3 | 1/2,1/2,1/2$)

(31) $3^* x,x+1,x,1/4,3/4$; $-1/4,1/4,3/4$

($3 | 1/2,1/2,1/2$)

(32) $3^* x+x+1,x; 3/4,-1/4,1/4$

($3 | 1/2,1/2,1/2$)

(33) $3^* x,x,x; 1/4,1/4,1/4$

($3 | 1/2,1/2,1/2$)

(34) $3^* x+1,x-1,x; 1/4,-1/4,3/4$

($3 | 1/2,1/2,1/2$)

(35) $3^* x,x+1,x; -1/4,3/4,1/4$

($3 | 1/2,1/2,1/2$)

(36) $3^* x+x+1,x,1; 3/4,3/4,-1/4$

($3 | 1/2,1/2,1/2$)

(37) $m^* x,x,z$

($m_{xy} | 0,0,0$)

(38) $m^* x,x,z$

($m_{xy} | 0,0,0$)

(39) $4^* x,0,z; 0,0,0$

($4z | 0,0,0$)

(40) $4^* x,0,0; 0,0,0$

($4z | 0,0,0$)

(41) $4^{-1} x,0,0; 0,0,0$

($4x | 0,0,0$)

(42) $m^* x,y,y$

($m_{yz} | 0,0,0$)

(43) $m^* x,y,y$

($m_{yz} | 0,0,0$)

(44) $4^* x,0,0; 0,0,0$

($4x | 0,0,0$)

(45) $4^* x,0,0; 0,0,0$

($4x | 0,0,0$)

(46) $m^* x,y,x$

($m_{xz} | 0,0,0$)

(47) $4^* x,y,0; 0,0,0$

($4y | 0,0,0$)

(48) $m^* x,y,x$

($m_{xz} | 0,0,0$)

For $(1,0,0)$ + set

(1) $t' (1,0,0)$

(1 | 1,0,0$)

(2) $2' 1/2,0,z$

($2z | 1,0,0$)

(3) $2' 1/2,y,0$

($2y | 1,0,0$)

(4) $2' (1,0,0) x,0,0$

($2x | 1,0,0$)

(5) $3^* (1/3,1/3,1/3)$

$x+2/3,x+1/3,x$

($3_{xyz} | 0,0,0$)

(6) $3^* (1/3,-1/3,1/3)$

$x+2/3,x-1/3,x$

($3_{xyz}^{-1} | 0,0,0$)

(7) $3^* (1/3,-1/3,1/3)$

$x+2/3,x-1/3,x$

($3_{xyz}^{-1} | 1,0,0$)

(8) $3^* (1/3,1/3,1/3)$

$x+2/3,x+1/3,x$

($3_{xyz} | 1,0,0$)

(9) $3^* (1/3,1/3,1/3)$

$x+1/3,x+1/3,x$

($3_{xyz}^{-1} | 0,0,0$)

(10) $3^* (1/3,-1/3,1/3)$

$x+1/3,x-1/3,x$

($3_{xyz}^{-1} | 0,0,0$)

(11) $3^* (1/3,1/3,-1/3)$

$x+1/3,x+1/3,x$

($3_{xyz} | 1,0,0$)

(12) $3^* (1/3,1/3,-1/3)$

$x+1/3,x+1/3,x$

($3_{xyz} | 1,0,0$)
Generators selected  

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1,0,0)' +</td>
</tr>
<tr>
<td>(2) x,y,z [u,v,w]</td>
<td>(1,0,0) + (0,0,0)' +</td>
</tr>
<tr>
<td>(4) x+1/2,x,1/4</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(8) z,x,y [w,u,v]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(3) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(10) y,z,x [v,w,u]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(11) y,z,x [v,w,u]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(12) y,z,x [v,w,u]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(13) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(14) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(0,0,0) + (1,0,0)</td>
</tr>
<tr>
<td>(15) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(0,0,0) + (1,0,0)</td>
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<tr>
<td>(16) y+1/2,x+1/2,z+1/2 [v,u,w]</td>
<td>(0,0,0) + (1,0,0)</td>
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Continued
Continued 224.7.1617  

<table>
<thead>
<tr>
<th>Expression</th>
<th>224.7.1617</th>
<th>$P_{F_n}n^3m'$</th>
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<tr>
<td>(37) $\bar{y}, x, z [v, u, w]$</td>
<td>(38) $y, x, z [v, u, w]$</td>
<td>(39) $\bar{y}, x, z [v, u, w]$</td>
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<tr>
<td>(41) $x, z, y [u, w, v]$</td>
<td>(42) $x, z, y [u, w, v]$</td>
<td>(43) $x, z, y [u, w, v]$</td>
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<tr>
<td>(45) $z, y, x [w, v, u]$</td>
<td>(46) $z, y, x [w, v, u]$</td>
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<td>$z+1/2, x+1/2, x+1/2 [w, u, u]$</td>
<td>$z+1/2, x+1/2, x+1/2 [w, u, u]$</td>
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<td>$3/4, y, y+1/2 [0, v, v]$</td>
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<td>$y, 3/4, y+1/2 [0, v, v]$</td>
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<tr>
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<td>$y+1/2, y, 3/4 [v, v, 0]$</td>
<td>$y+1/2, y, 3/4 [v, v, 0]$</td>
</tr>
<tr>
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<td>$3/4, y, y+1/2 [u, v, v]$</td>
<td>$3/4, y, y+1/2 [u, v, v]$</td>
</tr>
<tr>
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<td>$y+1/2, 3/4, y [v, u, v]$</td>
<td>$y+1/2, 3/4, y [v, u, v]$</td>
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<td>$y+1/2, y, 3/4 [v, v, u]$</td>
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</table>

224.7.1617 - 4 - 3721
Continued

\[
\begin{align*}
\bar{x} + 1/2, 1/2, 0 & \quad [0, v, w] \\
& \quad x + 1/2, 1/2, 0 \quad [0, v, \bar{w}] \\
& \quad 0, x + 1/2, 1/2 \quad [w, 0, v] \\
& \quad 0, x + 1/2, 1/2 \quad [w, 0, \bar{v}] \\
\bar{1}/2, 0, \bar{x} + 1/2 & \quad [v, w, 0] \\
& \quad 1/2, 0, x + 1/2 \quad [v, \bar{w}, 0] \\
& \quad 0, \bar{x}, 1/2 \quad [\bar{v}, 0, w] \\
& \quad 0, \bar{x}, 1/2 \quad [\bar{v}, 0, \bar{w}] \\
\bar{x}, 1/2, 0 & \quad [0, w, \bar{v}] \\
& \quad x, 1/2, 0 \quad [0, w, v] \\
& \quad 1/2, 0, x \quad [w, v, 0] \\
& \quad 1/2, 0, x \quad [w, v, \bar{w}] \\
24 & \quad g \quad 2m'm' \quad x, 0, 0 \quad [0, u, 0] \\
& \quad \bar{x}, 0, 0 \quad [\bar{u}, 0, 0] \\
& \quad 0, x, 0 \quad [0, u, 0] \\
& \quad 0, x, 0 \quad [0, \bar{u}, 0] \\
& \quad x + 1/2, 1/2, 1/2 \quad [u, 0, 0] \\
& \quad x + 1/2, 1/2, 1/2 \quad [\bar{u}, 0, 0] \\
& \quad 1/2, x + 1/2, 1/2 \quad [0, u, 0] \\
& \quad 1/2, x + 1/2, 1/2 \quad [0, \bar{u}, 0] \\
24 & \quad f \quad 2':2' \quad 1/4, 0, 1/2 \quad [0, v, v] \\
& \quad 3/4, 0, 1/2 \quad [0, v, \bar{v}] \\
& \quad 1/2, 1/4, 0 \quad [v, v, 0] \\
& \quad 0, 1/2, 1/4 \quad [v, v, \bar{v}] \\
& \quad 1/4, 1/2, 0 \quad [0, v, v] \\
& \quad 3/4, 1/2, 0 \quad [0, \bar{v}, v] \\
& \quad 0, 1/4, 1/2 \quad [v, v, 0] \\
& \quad 0, 1/4, 1/2 \quad [v, \bar{v}, v] \\
16 & \quad e \quad .3m' \quad x, x, x \quad [u, u, u] \\
& \quad \bar{x}, x, x \quad [\bar{u}, \bar{u}, \bar{u}] \\
& \quad \bar{x}, x, x \quad [\bar{u}, u, u] \\
& \quad \bar{x}, x, x \quad [u, u, u] \\
& \quad x + 1/2, x + 1/2, x + 1/2 \quad [\bar{u}, u, u] \\
& \quad x + 1/2, x + 1/2, x + 1/2 \quad [\bar{u}, \bar{u}, \bar{u}] \\
& \quad 1/2, x + 1/2, x + 1/2 \quad [u, u, u] \\
& \quad 1/2, x + 1/2, x + 1/2 \quad [u, \bar{u}, \bar{u}] \\
12 & \quad d \quad \bar{4}2'.m' \quad 0, 1/2, 1/2 \quad [u, 0, 0] \\
& \quad 1/2, 0, 1/2 \quad [0, u, 0] \\
& \quad 1/2, 1/2 \quad [0, 0, u] \\
& \quad 1/2, 1/2 \quad [0, 0, u] \\
& \quad 0, 1/2, 0 \quad [0, u, 0] \\
& \quad 1/2, 0, 0 \quad [u, 0, 0] \\
& \quad 0, 0, 1/2 \quad [0, 0, u] \\
8 & \quad c \quad .3'm' \quad 3/4, 3/4, 3/4 \quad [0, 0, 0] \\
& \quad 1/4, 1/4, 3/4 \quad [0, 0, 0] \\
& \quad 1/4, 3/4, 1/4 \quad [0, 0, 0] \\
& \quad 3/4, 1/4, 1/4 \quad [0, 0, 0] \\
8 & \quad b \quad .3'm' \quad 1/4, 1/4, 1/4 \quad [u, u, u] \\
& \quad 3/4, 3/4, 1/4 \quad [u, u, u] \\
& \quad 3/4, 1/4, 3/4 \quad [u, u, u] \\
& \quad 1/4, 3/4, 3/4 \quad [u, u, u] \\
4 & \quad a \quad \bar{4}3'm' \quad 0, 0, 0 \quad [0, 0, 0] \\
& \quad 1/2, 1/2, 1/2 \quad [0, 0, 0] \\

\textbf{Symmetry of Special Projections}

\begin{align*}
\text{Along } [0,0,1] & \quad \text{p4mm}
\quad a^* = (a - b)/2 \\
\quad \text{b}^* = (a + b)/2 \\
\text{Origin at } 0,0,2 \\
\text{Along } [1,1,1] & \quad \text{p6mm}
\quad a^* = (2a - b - c)/3 \\
\quad \text{b}^* = (-a + 2b - c)/3 \\
\text{Origin at } x,x,x \\
\text{Along } [1,1,0] & \quad \text{p}_{2}2\text{mm}
\quad a^* = (-a + b)/2 \\
\quad \text{b}^* = c \\
\text{Origin at } x-1/4,x+1/4,1/4
\end{align*}
Origin at center (m\(\bar{3}\)m)

Asymmetric unit 
0 \(\leq\) x \(\leq\) 1/2; 0 \(\leq\) y \(\leq\) 1/4; 0 \(\leq\) z \(\leq\) 1/4; y \(\leq\) min(x, 1/2-x); z \(\leq\) y

Vertices 0,0,0 1/2,0,0 1/4,1/4,0 1/4,1/4,1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1|0,0,0)

(2) 2 0,0,z
(2|0,0,0)

(3) 2 y,0,0
(2|0,0,0)

(4) 2 x,0,0
(2|0,0,0)

(5) 3' x,x,x
(3_{xyz}|0,0,0)

(6) 3' x,x,x
(3_{xyz}|0,0,0)

(7) 3' x,x,x
(3_{xyz}|0,0,0)

(8) 3' x,x,x
(3_{xyz}|0,0,0)

(9) 3' x,x,x
(3_{xyz}^{-1}|0,0,0)

(10) 3' x,x,x
(3_{xyz}^{-1}|0,0,0)

(11) 3' x,x,x
(3_{xyz}^{-1}|0,0,0)

(12) 3' x,x,x
(3_{xyz}^{-1}|0,0,0)
Continued

(13) 2 \(x, x, 0\)

(14) 2 \(x, x, 0\)

(15) 4\(^+\) 0, 0, 0

(16) 4\(^+\) 0, 0, 0

(2\(x_y\) 0, 0, 0)

(2\(x_y\) 0, 0, 0)

(4\(_x\) 0, 0, 0)

(4\(_x\) 0, 0, 0)

(17) 4\(^+\) 0, 0, 0

(18) 2 0, 0, 0

(19) 2 0, 0, 0

(20) 4\(^+\) 0, 0, 0

(4\(_x\) 0, 0, 0)

(4\(_x\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(21) 4\(^+\) 0, 0, 0

(22) 2 0, 0, 0

(23) 4\(^+\) 0, 0, 0

(24) 2 0, 0, 0

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(2\(_x\) 0, 0, 0)

(2\(_x\) 0, 0, 0)

(25) 1 0, 0, 0

(26) m 0, 0, 0

(27) m 0, 0, 0

(28) m 0, 0, 0

(1\(_x\) 0, 0, 0)

(1\(_x\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(3) 3\(^+\) x, x, x; 0, 0, 0

(3) 3\(^+\) x, x, x; 0, 0, 0

(3) 3\(^+\) x, x, x; 0, 0, 0

(3) 3\(^+\) x, x, x; 0, 0, 0

(3\(_xyz\) 0, 0, 0)

(3\(_xyz\) 0, 0, 0)

(3\(_xyz\) 0, 0, 0)

(3\(_xyz\) 0, 0, 0)

(37) m 0, 0, 0

(38) m 0, 0, 0

(39) 4\(^+\) 0, 0, 0

(40) 4\(^+\) 0, 0, 0

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(41) 4\(^+\) x, 0, 0; 0, 0, 0

(42) m 0, 0, 0

(43) m 0, 0, 0

(44) 4\(^+\) x, 0, 0; 0, 0, 0

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(45) 4\(^+\) 0, y, 0; 0, 0, 0

(46) m 0, 0, 0

(47) 4\(^+\) 0, y, 0; 0, 0, 0

(48) m 0, 0, 0

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

(4\(_y\) 0, 0, 0)

For \((0,1/2,1/2) + \text{set}\)

(1) t 0, 1/2, 1/2

(2) 2 0, 0, 1/2

(3) 2 0, 1/2, 0

(4) 2 0, 1/2, 1/2

(1\(_x\) 0, 1/2, 1/2)

(2\(_x\) 0, 1/2, 1/2)

(3\(_x\) 0, 1/2, 1/2)

(4\(_x\) 0, 1/2, 1/2)

(5) 3\(^+\) 1/3, 1/3, 1/3

(6) 3\(^+\) 1/3, 1/3, 1/3

(7) 3\(^+\) 1/3, 1/3, 1/3

(8) 3\(^+\) 1/3, 1/3, 1/3

x-1/3, x-1/3, x

x-1/3, x-1/3, x

x-1/3, x-1/3, x

x-1/3, x-1/3, x

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(9) 3\(^+\) 1/3, 1/3, 1/3

(10) 3\(^+\) 1/3, 1/3, 1/3

(11) 3\(^+\) 1/3, 1/3, 1/3

(12) 3\(^+\) 1/3, 1/3, 1/3

x-1/3, x-1/3, x

x-1/3, x-1/3, x

x-1/3, x-1/3, x

x-1/3, x-1/3, x

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(13) 2 0, 1/4, 1/4

(14) 2 0, 1/4, 1/4

(15) 4\(^+\) 0, 0, 1/2

(16) 4\(^+\) 0, 0, 1/2

(2\(_x\) 0, 1/2, 1/2)

(2\(_x\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(17) 4\(^+\) 0, 1/2, 0

(18) 2 0, 1/2, 0

(19) 2 0, 1/2, 0

(20) 4\(^+\) 0, 1/2, 0

(4\(_y\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(21) 4\(^+\) 0, 1/2, 0

(22) 2 0, 1/2, 0

(23) 4\(^+\) 0, 1/2, 0

(24) 2 0, 1/2, 0

(4\(_y\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(4\(_y\) 0, 1/2, 1/2)

(25) t 0, 1/4, 1/4

(26) b 0, 1/2, 0

(27) c 0, 1/2, 0

(28) n 0, 1/2, 1/2

(1\(_x\) 0, 1/2, 1/2)

(1\(_x\) 0, 1/2, 1/2)

(1\(_x\) 0, 1/2, 1/2)

(1\(_x\) 0, 1/2, 1/2)

(29) 3\(^+\) x+1/2, x

(30) 3\(^+\) x+1/2, x

(31) 3\(^+\) x+1/2, x

(32) 3\(^+\) x+1/2, x

0, 1/2, 0

0, 1/2, 0

0, 1/2, 0

0, 1/2, 0

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)

(3\(_xyz\) 0, 1/2, 1/2)
Continued 225.1.1618

(33) \(3^+ \cdot x-1/2, x-1/2, x; 0, 0, 1/2\)

(34) \(3^- \cdot x+1/2, x-1/2, x; 0, 0, 1/2\)

(35) \(3^- \cdot x-1/2, x+1/2, x; 1/2, 1/2, 0\)

(36) \(3^- \cdot x+1/2, x+1/2, x; 1/2, 1/2, 0\)

(37) \(g (-1/4, 1/4, 1/2) \cdot x+1/4, x, z \cdot (m_x y, 0, 1/2, 1/2)\)

(38) \(g (1/4, 1/4, 1/2) \cdot x-1/4, x, z \cdot (m_x y, 0, 1/2, 1/2)\)

(39) \(g (-1/4, 1/4, 1/2) \cdot x-1/4, x, z \cdot (m_x y, 0, 1/2, 1/2)\)

(40) \(4^+ \cdot 1/4, 1/4, z; 1/4, 1/4, 1/4 \cdot (m_x y, 0, 1/2, 1/2)\)

(41) \(4^- \cdot x, 0, 1/2; 0, 0, 1/2\)

(42) \(m \cdot x, y+1/2, y \cdot (m_{y z}, 0, 1/2, 1/2)\)

(43) \(g (0, 0, 1/2) \cdot x, y, y \cdot (m_{y z}, 0, 1/2, 1/2)\)

(44) \(4^+ \cdot x, 1/2, 0; 0, 1/2, 0 \cdot (m_{y z}, 0, 1/2, 1/2)\)

(45) \(4^- \cdot -1/4, 1/4, 1/4; -1/4, 1/4, 1/4\)

(46) \(g (-1/4, 1/4, 1/4) \cdot x+1/4, y, x \cdot (m_x z, 0, 1/2, 1/2)\)

(47) \(4^- \cdot 1/4, y, 1/4; 1/4, 1/4, 1/4 \cdot (m_{x z}, 0, 1/2, 1/2)\)

(48) \(g (1/4, 1/2, 1/4) \cdot x-1/4, y, x \cdot (m_x z, 0, 1/2, 1/2)\)

For \((1/2,0,1/2) + \) set

(1) \(t (1/2,0,1/2)\)

(2) \(2 \cdot (0,0,1/2) \cdot 1/4,0,z\)

(3) \(2 \cdot 1/4,y,1/4\)

(4) \(2 \cdot (1/2,0,0) \cdot x,0,1/2\)

(2_1 \cdot 1/2,0,1/2)\)

(2_2 \cdot 1/2,0,1/2)\)

(5) \(3^+ \cdot (1/3,1/3,1/3) \cdot x+1/6,x-1/6,x\)

(6) \(3^+ \cdot (1/3,1/3,1/3) \cdot x+1/6,x+1/6,x\)

(7) \(3^+ \cdot x+1/2,x-1/2,x\)

(8) \(3^- \cdot x+1/2,x+1/2,x\)

(9) \(3 \cdot (1/3,1/3,1/3) \cdot x+1/6,x-1/6,x\)

(10) \(3^- \cdot x+1/2,x,x\)

(11) \(3^- \cdot x+1/2,x, x\)

(12) \(3 \cdot (1/3,1/3,1/3) \cdot x+1/6,x+1/3,x\)

(13) \(2 \cdot (1/4,1/4,0) \cdot x,x-1/4,1/4\)

(14) \(2 \cdot (1/4,1/4,0) \cdot x,x+1/4,1/4\)

(15) \(4 \cdot (0,0,1/2) \cdot 1/4,-1/4,z\)

(16) \(4^- \cdot (0,0,1/2) \cdot 1/4,1/4,z\)

(17) \(4^- \cdot (1/2,0,0) \cdot x,1/4,1/4\)

(18) \(2 \cdot (0,1/4,1/4) \cdot 1/4,y-1/4,y\)

(19) \(2 \cdot (0,-1/2,1/2) \cdot 1/4,y+1/4,y\)

(20) \(4^- \cdot (1/2,0,0) \cdot x,-1/4,1/4\)

(21) \(4^- \cdot 1/2,y,0\)

(22) \(2 \cdot (1/2,0,1/2) \cdot x,0,x\)

(23) \(4^- \cdot y,0,1/2\)

(24) \(2 \cdot x+1/2,0,x\)

(25) \(a \cdot 1/4,0,1/4\)

(26) \(a \cdot (1/2,0,0) \cdot x,y,1/4\)

(27) \(n \cdot (1/2,0,1/2) \cdot x,0,z\)

(28) \(c \cdot (0,0,1/2) \cdot 1/4,y,z\)

(29) \(3^- \cdot x-1/2,x+1/2,x; 0,0,1/2\)

(30) \(3^- \cdot x-1/2,x+1/2,x; 0,0,1/2\)

(31) \(3^+ \cdot x+1/2,x+1/2,x; 1/2,1/2,0\)

(32) \(3^- \cdot x+1/2,x+1/2,x; 1/2,1/2,0\)

(33) \(3^- \cdot x+1/2,x,x; 1/2,0,0\)

(34) \(3^- \cdot x+1/2,x,x; 1/2,0,0\)

(35) \(3^- \cdot x+1/2,x,x; 1/2,0,0\)

(36) \(3^- \cdot x+1/2,x,x; 1/2,0,0\)

(37) \(g (1/4,-1/4,1/2) \cdot x+1/4,x, z \cdot (m_x y, 1/2,0,1/2)\)

(38) \(g (1/4,1/4,1/2) \cdot x+1/4,x, z \cdot (m_x y, 1/2,0,1/2)\)

(39) \(4^- \cdot 1/4,1/4,z; 1/4,1/4,1/4 \cdot (m_x y, 1/2,0,1/2)\)

(40) \(4^- \cdot 1/4,-1/4,z; 1/4,-1/4,1/4 \cdot (m_x y, 1/2,0,1/2)\)

(41) \(4^- \cdot x,-1/4,1/4; 1/4,-1/4,1/4\)

(42) \(g (1/2,-1/4,1/4) \cdot x,y+1/4,y \cdot (m_y z, 1/2,0,1/2)\)

(43) \(g (1/2,1/4,1/4) \cdot x,y-1/4,y \cdot (m_y z, 1/2,0,1/2)\)

(44) \(4^- \cdot x,1/4,1/4; 1/4,1/4,1/4 \cdot (m_y z, 1/2,0,1/2)\)

(45) \(4^- \cdot 0,1/2,0,0\)

(46) \(m \cdot x+1/2,y,x \cdot (m_z, 1/2,0,1/2)\)

(47) \(4^- \cdot 1/2,y,0; 1/2,0,0\)

(48) \(g (1/2,0,1/2) \cdot x, y, x \cdot (m_z, 1/2,0,1/2)\)
Continued 225.1.1618 Fm3m

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(2) 2 1/4,1/4,z
(3) 2 (0,1/2,0) 1/4,y,0
(4) 2 (1/2,0,0) x,1/4,0
(5) 3+ (1/3,1/3,1/3)
    x+1/6,x+1/3,x
(3_{xyz}^{-1}|1/2,1/2,0)
(6) 3+ x+1/2,x,x
(7) 3+ x+1/2,x,x
(8) 3+ (1/3,1/3,-1/3)
    x+1/6,x+1/3,x
(3_{xyz}^{-1}|1/2,1/2,0)
(9) 3+ (1/3,1/3,1/3)
    x+1/3,x+1/6,x
(3_{xyz}^{-1}|1/2,1/2,0)
(10) 3+ x,x+1/2,x
(11) 3+ (1/3,1/3,-1/3)
    x+1/3,x+1/6,x
(12) 3+ x,x+1/2,x
(13) 2 (1/2,1/2,0)
    x,x,0
(14) 2 x,x+1/2,0
(15) 4+ 1/2,0,z
(16) 4+ 0,1/2,z
(17) 4+ (1/2,0,0)
    x,1/4,-1/4
(4_{y}^{-1}|1/2,1/2,0)
(18) 2 (0,1/4,1/4)
    1/4,y+1/4,y
(2_{xy}|1/2,1/2,0)
(19) 2 (0,1/4,-1/4)
    1/4,y+1/4,y
(2_{yz}|1/2,1/2,0)
(20) 4+ (1/2,0,0)
    x,1/4,1/4
(4_{z}^{-1}|1/2,1/2,0)
(21) 4+ (0,1/2,0)
    1/4,y,-1/4
(4_{y}^{-1}|1/2,1/2,0)
(22) 2 (1/4,0,1/4)
    x+1/4,1/4,x
(2_{xy}|1/2,1/2,0)
(23) 4+ (0,1/2,0)
    1/4,y,1/4
(4_{y}^{-1}|1/2,1/2,0)
(24) 2 (1/4,0,-1/4)
    x+1/4,1/4,x
(2_{xz}|1/2,1/2,0)
(25) 1/4,1/4,0
(1/2,1/2,0)
(26) n (1/2,1/2,0)
    x,y,0
(27) a (1/2,0,0)
    x,1/4,z
(28) b (0,1/2,0)
    1/4,y,z
(29) 3+ x+1/2,x,x;
    1/2,0
(3_{xyz}^{-1}|1/2,1/2,0)
(30) 3+ x-1/2,x+1,x;
    0,1/2,1/2
(3_{xyz}^{-1}|1/2,1/2,0)
(31) 3+ x-1/2,x+1,x;
(3_{xyz}^{-1}|1/2,1/2,0)
(32) 3+ x+1/2,x,x;
(3_{xyz}^{-1}|1/2,1/2,0)
(33) 3+ x,x+1/2,x;
    0,1/2,0
(3_{xyz}^{-1}|1/2,1/2,0)
(34) 3+ x+1,x-1/2,x;
    0,1/2,0
(3_{xyz}^{-1}|1/2,1/2,0)
(35) 3+ x,x+1/2,x;
(3_{xyz}^{-1}|1/2,1/2,0)
(36) 3+ x+1,x-1/2,x;
(3_{xyz}^{-1}|1/2,1/2,0)
(37) m x+1/2,x,z
(3_{xyz}^{-1}|1/2,1/2,0)
(38) g (1/2,1/2,0)
    x,x,z
(39) 4+ 0,1/2,z; 0,1/2,0
(4_{y}^{-1}|1/2,1/2,0)
(40) 4+ 1/2,0,z; 1/2,0,0
(4_{z}^{-1}|1/2,1/2,0)
(41) 4+ x,1/4,1/4;
    1/4,1/4,1/4
(4_{y}^{-1}|1/2,1/2,0)
(42) g (1/2,1/2,0)
    x,y+1/4,y
(43) g (1/2,1/4,1/4)
    x,y+1/4,y
(44) 4+ x,1/4,-1/4;
    1/4,1/4,1/4
(4_{x}^{-1}|1/2,1/2,0)
(45) 4+ 1/4,y,1/4;
    1/4,1/4,1/4
(4_{y}^{-1}|1/2,1/2,0)
(46) g (1/2,1/2,0)
    x+1/4,y,x
(47) 4+ 1/4,y,-1/4;
    1/4,1/4,1/4
(4_{y}^{-1}|1/2,1/2,0)
(48) g (1/4,1/2,1/4)
    x+1/4,y,x
(4_{x}^{-1}|1/2,1/2,0)

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

192 I 1

(1) x,y,z [u,v,w]
(2) x, y, z [u, v, w]
(3) x, y, z [u, v, w]
(4) x, y, z [u, v, w]
(5) z, x, y [w, u, v]
(6) z, x, y [w, u, v]
(7) z, x, y [w, u, v]
(8) z, x, y [w, u, v]

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(9) y,z,x [v,w,u]  
(10) y,z,x [v,w,u]  
(11) y,z,x [v,w,u]  
(12) y,z,x [v,w,u]  
(13) y,x,z [v,u,w]  
(14) y,x,z [v,u,w]  
(15) y,x,z [v,u,w]  
(16) y,x,z [v,u,w]  
(17) x,z,y [u,w,v]  
(18) x,z,y [u,w,v]  
(19) x,z,y [u,w,v]  
(20) x,z,y [u,w,v]  
(21) z,y,x [w,v,u]  
(22) z,y,x [w,v,u]  
(23) z,y,x [w,v,u]  
(24) z,y,x [w,v,u]  
(25) x,y,z [u,v,w]  
(26) x,y,z [u,v,w]  
(27) x,y,z [u,v,w]  
(28) x,y,z [u,v,w]  
(29) z,x,y [w,u,v]  
(30) z,x,y [w,u,v]  
(31) z,x,y [w,u,v]  
(32) z,x,y [w,u,v]  
(33) y,z,x [v,w,u]  
(34) y,z,x [v,w,u]  
(35) y,z,x [v,w,u]  
(36) y,z,x [v,w,u]  
(37) y,x,z [v,u,w]  
(38) y,x,z [v,u,w]  
(39) y,x,z [v,u,w]  
(40) y,x,z [v,u,w]  
(41) x,z,y [u,w,v]  
(42) x,z,y [u,w,v]  
(43) x,z,y [u,w,v]  
(44) x,z,y [u,w,v]  
(45) z,y,x [w,v,u]  
(46) z,y,x [w,v,u]  
(47) z,y,x [w,v,u]  
(48) z,y,x [w,v,u]  

96  k  ..m  x,x,z [u,u,0]  
z,x,x [0,u,u]  
x,z,x [u,0,u]  
x,x,z [u,u,0]  

96  j  m..  0,y,z [u,0,u]  
z,0,y [0,u,0]  
y,z,0 [0,u,u]  
y,0,z [0,u,0]  

48  i  m.m2  1/2,y,y [0,0,0]  
y,1/2,y [0,0,0]  
y,y,1/2 [0,0,0]  

48  h  m.m2  0,y,y [0,0,0]  
y,0,y [0,0,0]  
y,y,0 [0,0,0]  

225.1.1618 - 5 - 3727
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Origin</th>
<th>a*</th>
<th>b*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Along [0,0,1]</td>
<td>p4mm1'</td>
<td>( \frac{a}{2} )</td>
<td>( \frac{b}{2} )</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along [1,1,1]</td>
<td>p6'm'm</td>
<td>( \frac{2a - b - c}{6} )</td>
<td>( \frac{-a + 2b - c}{6} )</td>
</tr>
<tr>
<td>Origin at x,x,x</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Along [1,1,0]</td>
<td>c2mm1'</td>
<td>( \frac{-a + b}{2} )</td>
<td>( c )</td>
</tr>
<tr>
<td>Origin at x,x,0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Origin at center ($m\bar{3}m'$)

Asymmetric unit

$0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad z \leq y$

Vertices

$0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,0 \quad 1/4,1/4,1/4$

Symmetry Operations

For $(0,0,0) + \text{set}$

1. $1$
2. $2 \cdot 0,0,z$
3. $2 \cdot 0,y,0$
4. $2 \cdot x,0,0$
5. $3^+ x,x,x$
6. $3^+ x,x,x$
7. $3^+ x,x,x$
8. $3^+ x,x,x$
9. $3^- x,x,x$
10. $3^- x,x,x$
11. $3^- x,x,x$
12. $3^- x,x,x$

$Fm\bar{3}m'$ $m\bar{3}m'$ Cubic

225.2.1619 225.2.1619
Continued

<table>
<thead>
<tr>
<th>(13) 2  x,x,0</th>
<th>(14) 2  x,x,0</th>
<th>(15) 4  0,0,z</th>
<th>(16) 4  0,0,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>2xy</td>
<td>0,0,0)</td>
<td>(2xy</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(17) 4  x,0,0</th>
<th>(18) 2  0,y,y</th>
<th>(19) 2  0,y,y</th>
<th>(20) 4  x,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>4xz</td>
<td>0,0,0)</td>
<td>(2yz</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(21) 4  0,y,0</th>
<th>(22) 2  x,0,x</th>
<th>(23) 4  0,y,0</th>
<th>(24) 2  x,0,x</th>
</tr>
</thead>
<tbody>
<tr>
<td>4y</td>
<td>0,0,0)</td>
<td>(2xz</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(25) 1  0,0,0</th>
<th>(26) m  x,y,0</th>
<th>(27) m  x,0,z</th>
<th>(28) m  0,y,z</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10,0,0,0)</td>
<td>(mxy</td>
<td>0,0,0)</td>
<td>(mx</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(29) 3  x,x;x,0,0,0</th>
<th>(30) 3  x,x;x,0,0,0</th>
<th>(31) 3  x,x,x;0,0,0</th>
<th>(32) 3  x,x,x;0,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3)xyz</td>
<td>0,0,0)</td>
<td>(3)xyz</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(33) 3  x,x,x;0,0,0</th>
<th>(34) 3  x,x,x;0,0,0</th>
<th>(35) 3  x,x,x;0,0,0</th>
<th>(36) 3  x,x,x;0,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>3xyz</td>
<td>0,0,0)</td>
<td>(3xyz</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(37) m  x,x,z</th>
<th>(38) m  x,x,z</th>
<th>(39) m  x,y,y</th>
<th>(40) m  0,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(mxy</td>
<td>0,0,0)</td>
<td>(mxy</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(41) 4  x,0,0;0,0,0</th>
<th>(42) m  x,y,y</th>
<th>(43) m  x,y,y</th>
<th>(44) m  0,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4y</td>
<td>0,0,0)</td>
<td>(mxy</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(45) 4  0,y,0;0,0,0</th>
<th>(46) m  x,y,x</th>
<th>(47) m  0,0,0</th>
<th>(48) m  0,0,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>4y</td>
<td>0,0,0)</td>
<td>(mxy</td>
<td>0,0,0)</td>
</tr>
</tbody>
</table>

For (0,1/2,1/2) + set

<table>
<thead>
<tr>
<th>(1) t  (0,1/2,1/2)</th>
<th>(2) 2  (0,0,1/2)</th>
<th>(3) 2  (0,1/2,0)</th>
<th>(4) 2  x,1/4,1/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,0,2,1/2)</td>
<td>(2z</td>
<td>0,1/2,1/2)</td>
<td>(2y</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(5) 3  (1/3,1/3,1/3)</th>
<th>(6) 3  (0,1/2,1/2)</th>
<th>(7) 3  (-1/3,1/3,1/3)</th>
<th>(8) 3  x,x+1/2,x</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3xyz</td>
<td>0,1/2,1/2)</td>
<td>(3xyz</td>
<td>0,1/2,1/2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(9) 3  (1/3,1/3,1/3)</th>
<th>(10) 3  (0,1/2,1/2)</th>
<th>(11) 3  (0,1/2,1/2)</th>
<th>(12) 3  x,x+1/2,x</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3xyz</td>
<td>0,1/2,1/2)</td>
<td>(3xyz</td>
<td>0,1/2,1/2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(13) 2  (1/4,1/4,0)</th>
<th>(14) 2  (1/4,1/4,0)</th>
<th>(15) 4  (0,0,1/2)</th>
<th>(16) 4  (0,0,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2xy</td>
<td>0,1/2,1/2)</td>
<td>(2xy</td>
<td>0,1/2,1/2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(17) 4  x,1/2,0</th>
<th>(18) 2  (0,1/2,1/2)</th>
<th>(19) 2  (0,1/2,1/2)</th>
<th>(20) 4  x,1/2,0</th>
</tr>
</thead>
<tbody>
<tr>
<td>4y</td>
<td>0,1/2,1/2)</td>
<td>(2y</td>
<td>0,1/2,1/2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(21) 4  (0,1/2,0)</th>
<th>(22) 2  (1/4,0,1/4)</th>
<th>(23) 4  (0,1/2,0)</th>
<th>(24) 4  (1/4,0,1/4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4z</td>
<td>0,1/2,1/2)</td>
<td>(2yz</td>
<td>0,1/2,1/2)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(25) 1  (0,1/2,1/2)</th>
<th>(26) b  (0,1/2,0)</th>
<th>(27) c  (0,0,1/2)</th>
<th>(28) n  (0,1/2,1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10,0,1/2,1/2)</td>
<td>(mz</td>
<td>0,1/2,1/2)</td>
<td>(mx</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(29) 3  x,x+1/2,x</th>
<th>(30) 3  x,x+1/2,x</th>
<th>(31) 3  x,x+1/2,x</th>
<th>(32) 3  x,x+1/2,x</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3xyz</td>
<td>0,1/2,1/2)</td>
<td>(3xyz</td>
<td>0,1/2,1/2)</td>
</tr>
</tbody>
</table>
Continued 225.2.1619 Fm3m1'
Continued

For $(1/2,1/2,0) + \text{set}$

$(1) \ t (1/2,1/2,0)$
$(1/2,1/2,0)$

$(5) \ 3^* (1/3,1/3,1/3)$
$x+1/6,x+1/3,x$
$(3_{xyz}|_{1/2,1/2,0})$

$(9) \ 3^* (1/3,1/3,1/3)$
$x+1/3,x+1/6,x$
$(3_{xyz}|^{-1}_{1/2,1/2,0})$

$(13) \ 2 (1/2,1/2,0)$
$x,x,0$
$(2_{xy}|_{1/2,1/2,0})$

$(17) \ 4^* (1/2,0,0)$
$x,1/4,-1/4$
$(4_{x}|_{1/2,1/2,0})$

$(25) \ 1/4,1/4,0$
$(1/4,1/2,0)$

$(29) \ 3^* \ x+1/2,x,x$
$1/2,0$
$(3_{xyz}|_{1/2,1/2,0})$

$(33) \ 3^* \ x,x+1/2,x$
$0,1/2,0$
$(3_{xyz}|^{-1}_{1/2,1/2,0})$

$(37) \ m \ x+1/2,x,z$
$(m_{xy}|_{1/2,1/2,0})$

$(41) \ 4^* \ x,1/4,1/4; 1/4,1/4,1/4$
$(4_{x}|^{-1}_{1/2,1/2,0})$

$(45) \ 4^* \ 1/4,1/4,1/4; 1/4,1/4,1/4$
$(4_{y}|_{1/2,1/2,0})$

For $(0,0,0)^\prime + \text{set}$

$(1) \ 1^\prime$
$(1 | 0,0,0)^\prime$

$(5) \ 3^* \ x,x,x$
$(3_{xyz}|_{0,0,0})^\prime$

$(9) \ 3^* \ x,x,x$
$(3_{xyz}|^{-1}_{0,0,0})^\prime$

$(13) \ 2^* \ x,x,0$
$(2_{xy}|_{0,0,0})^\prime$

$(17) \ 4^* \ x,0,0$
$(4_{x}|^{-1}_{0,0,0})^\prime$
Continued

<table>
<thead>
<tr>
<th>Generators selected</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0,0,0) + (0,1/2,1/2,0) + (1/2,0,1/2,0) + (1/2,1/2,0) + (0,0,0)' + (0,1/2,1/2,0)' + (1/2,0,1/2,0)' + (1/2,1/2,0)' +</td>
</tr>
<tr>
<td>(1) x,y,z [0,0,0]</td>
<td>(2) x,y,z [0,0,0]</td>
</tr>
<tr>
<td>(5) z,x,y [0,0,0]</td>
<td>(6) z,x,y [0,0,0]</td>
</tr>
<tr>
<td>(9) y,z,x [0,0,0]</td>
<td>(10) y,z,x [0,0,0]</td>
</tr>
<tr>
<td>(13) y,x,z [0,0,0]</td>
<td>(14) y,x,z [0,0,0]</td>
</tr>
<tr>
<td>(17) x,z,y [0,0,0]</td>
<td>(18) x,z,y [0,0,0]</td>
</tr>
<tr>
<td>(21) z,y,x [0,0,0]</td>
<td>(22) z,y,x [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(4) x,y,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(8) z,x,y [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(12) y,z,x [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(16) y,x,z [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(20) x,z,y [0,0,0]</td>
</tr>
<tr>
<td></td>
<td>(24) z,y,x [0,0,0]</td>
</tr>
</tbody>
</table>

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Continued

| 24 | e | 4m.m1' x,0,0 [0,0,0] | $\bar{x},0,0 [0,0,0]$ | 0,x,0 [0,0,0] |
| 24 | d | m.mm1' 0,1/4,1/4 [0,0,0] | 0,3/4,1/4 [0,0,0] | 1/4,0,1/4 [0,0,0] |

| 8 | c | $\overline{4}3m1'$ 1/4,1/4,1/4 [0,0,0] | 1/4,1/4,3/4 [0,0,0] |
| 4 | b | m3m1' 1/2,1/2,1/2 [0,0,0] |
| 4 | a | m3m1' 0,0,0 [0,0,0] |

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Along [0,0,1] p4mm1'</th>
<th>Along [1,1,1] p6mm1'</th>
<th>Along [1,1,0] c2mm1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a^* = a/2$</td>
<td>$a^* = (2a - b - c)/6$</td>
<td>$a^* = (-a + b)/2$</td>
</tr>
<tr>
<td>$b^* = b/2$</td>
<td>$b^* = (-a + 2b - c)/6$</td>
<td>$b^* = c$</td>
</tr>
<tr>
<td>Origin at 0,0,z</td>
<td>Origin at x,x,x</td>
<td>Origin at x,x,0</td>
</tr>
</tbody>
</table>
Fm'3'm  
225.3.1620  

Asymmetric unit:  

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/4; \quad y \leq \min(x, 1/2-x); \quad z \leq y \]

Vertices:  

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/4,1/4,0 & \quad 1/4,1/4,1/4
\end{align*}
\]

Symmetry Operations:  

For \((0,0,0) + \) set:

\[
\begin{align*}
(1) & \quad 1 \\
(1,0,0,0) & \quad (2) & \quad 0,0,z \\
(2,0,0,0) & \quad (3) & \quad 0,y,0 \\
(2,y,0,0) & \quad & \quad (4) & \quad 0,x,0 \\
(2,0,0,0) & \quad (5) & \quad 1,x,x \\
(3_{xyz}|0,0,0) & \quad (6) & \quad x,x,x \\
(3_{xyz}^{-1}|0,0,0) & \quad (7) & \quad x,x,x \\
(3_{xyz}^{-1}|0,0,0) & \quad & \quad (8) & \quad x,x,x \\
(3_{xyz}^{-1}|0,0,0) & \quad (9) & \quad x,x,x \\
(3_{xyz}^{-1}|0,0,0) & \quad (10) & \quad x,x,x \\
(3_{xyz}^{-1}|0,0,0) & \quad (11) & \quad x,x,x \\
(3_{xyz}^{-1}|0,0,0) & \quad & \quad (12) & \quad x,x,x \\
(3_{xyz}^{-1}|0,0,0)
\end{align*}
\]
Continued 225.3.1620 Fm'3'm

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
  (1/2,1/2,0)

(5) 3* (1/3,1/3,1/3)
    x+1/6,x+1/3,x
    (3_{xyz}|1/2,1/2,0)

(9) 3* (1/3,1/3,1/3)
    x+1/3,x+1/6,x
    (3_{xyz}|1/2,1/2,0)

(13) 2' (1/2,1/2,0)
     x,x,0
     (2_{xy}|1/2,1/2,0)

(17) 4' (1/2,0,0) x,1/4,-1/4
     (4_{y}|1/2,1/2,0)

(21) 4' (0,1/2,0) 1/4,y,-1/4
     (4_{y}|1/2,1/2,0)

(25) 1' 1/4,1/4,0
     (1'|1/2,1/2,0)

(29) 3' x+1/2,x,x;
     (3_{xyz}|1/2,1/2,0)

(33) 3' x,x+1/2; x;
     (3_{xyz}|1/2,1/2,0)

(37) m x+1/2,x,z
     (m_{xy}|1/2,1/2,0)

(41) 4' x,1/4,1/4; 1/4,1/4,1/4
     (4_{y}|1/2,1/2,0)

(45) 4' 1/4,y,1/4; 1/4,1/4,1/4
     (4_{y}|1/2,1/2,0)

Generators selected  (1); t(1/0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

192  I  1

0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) x,y,z [u,v,w]
(4) x,y,z [u,v,w]
(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]
Continued 225.3.1620

(9) \( y, z, x \) [v, w, u]

(10) \( \bar{y}, z, x \) [v, w, u]

(11) \( y, z, x \) [v, w, u]

(12) \( \bar{y}, z, x \) [v, w, u]

(13) \( y, x, z \) [v, u, w]

(14) \( \bar{y}, x, z \) [v, u, w]

(15) \( y, x, z \) [v, u, w]

(16) \( \bar{y}, x, z \) [v, u, w]

(17) \( x, z, y \) [u, w, v]

(18) \( \bar{x}, z, y \) [u, w, v]

(19) \( x, z, y \) [u, w, v]

(20) \( \bar{x}, z, y \) [u, w, v]

(21) \( z, y, x \) [w, v, u]

(22) \( \bar{z}, y, x \) [w, v, u]

(23) \( z, y, x \) [w, v, u]

(24) \( \bar{z}, y, x \) [w, v, u]

(25) \( x, y, z \) [u, v, w]

(26) \( \bar{x}, y, z \) [u, v, w]

(27) \( x, y, z \) [u, v, w]

(28) \( \bar{x}, y, z \) [u, v, w]

(29) \( z, x, y \) [w, u, v]

(30) \( \bar{z}, x, y \) [w, u, v]

(31) \( z, x, y \) [w, u, v]

(32) \( \bar{z}, x, y \) [w, u, v]

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(34) \( \bar{y}, z, x \) [v, w, u]

(35) \( y, z, x \) [v, w, u]

(36) \( \bar{y}, z, x \) [v, w, u]

(37) \( y, x, z \) [v, u, w]

(38) \( \bar{y}, x, z \) [v, u, w]

(39) \( y, x, z \) [v, u, w]

(40) \( \bar{y}, x, z \) [v, u, w]

(41) \( x, z, y \) [u, w, v]

(42) \( \bar{x}, z, y \) [u, w, v]

(43) \( x, z, y \) [u, w, v]

(44) \( \bar{x}, z, y \) [u, w, v]

(45) \( z, y, x \) [w, v, u]

(46) \( \bar{z}, y, x \) [w, v, u]

(47) \( z, y, x \) [w, v, u]

(48) \( \bar{z}, y, x \) [w, v, u]

96 \( k \) \(...

x, x, z [u, u, 0]

z, x, x [0, u, 0]

x, x, z [u, 0, u]

x, x, z [u, u, 0]

x, x, x [u, u, 0]

z, x, x [0, u, u]

x, x, x [0, u, 0]

96 \( j \) \(...

0, y, z [0, v, w]

0, y, z [0, v, w]

0, y, z [0, v, w]

0, y, z [0, v, w]

0, z, 0 [w, 0, v]

z, 0, y [w, 0, v]

y, z, 0 [v, w, 0]

0, z, 0 [v, w, 0]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

48 \( i \) \(...

1/2, y, y [0, v, w]

1/2, y, y [0, v, w]

1/2, y, y [0, v, w]

1/2, y, y [0, v, w]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

48 \( h \) \(...

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

0, y, 0 [w, 0, v]

225.3.1620 - 5 - 3742
### Symmetry of Special Projections

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<th>g</th>
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<td>1/4,3/4,x [0,0,0]</td>
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<td>f</td>
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<td>e</td>
<td>4'm'.m</td>
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<td>m'3'm</td>
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</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**: \( p4'm'm \)  
  \( a^* = a/2 \quad b^* = b/2 \)  
  Origin at 0,0,z

- **Along [1,1,1]**: \( p6mm \)  
  \( a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6 \)  
  Origin at x,x,x

- **Along [1,1,0]**: \( c2mm1\)'  
  \( a^* = (-a + b)/2 \quad b^* = c \)  
  Origin at x,x,0
Origin at center (m\overline{3}m')

Asymmetric unit  
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/4; 0 ≤ z ≤ 1/4; y ≤ min(x, 1/2-x); z ≤ y

Vertices  
0,0,0 1/2,0,0 1/4,1/4,0 1/4,1/4,1/4

Symmetry Operations

For (0,0,0) + set

(1) 1  
(2) 2  0,0,z  
(3) 2  0,y,0  
(4) 2  x,0,0  

(5) 3'  x,x,x  
(6) 3'  x,x,x  
(7) 3'  x,x,x  
(8) 3'  x,x,x

(3_{xyz})|0,0,0)  
(3_{xyz})|0,0,0)  
(3_{xyz})|0,0,0)  
(3_{xyz})|0,0,0)

(9) 3'  x,x,x  
(10) 3'  x,x,x  
(11) 3'  x,x,x  
(12) 3'  x,x,x

(3_{xyz}^{-1})|0,0,0)  
(3_{xyz}^{-1})|0,0,0)  
(3_{xyz}^{-1})|0,0,0)  
(3_{xyz}^{-1})|0,0,0)
Continued 

For (0,1/2,1/2) + set

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<tr>
<th>225.4.1621</th>
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</thead>
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<table>
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<tr>
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<td>14</td>
<td>2’ x,x,0</td>
<td>21</td>
<td>4‘+ 0,0,0</td>
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<td>15</td>
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<td>22</td>
<td>2’ x,0,0</td>
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<td>(4z'</td>
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<td>16</td>
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For (0,1/2,1/2) + set

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<td>3‘+ 0,0,0</td>
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For (0,1/2,1/2) + set

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For (0,1/2,1/2) + set
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<th>Formula</th>
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<td>34</td>
<td>(3^* x+1/2, x-1/2, x; 0, 0, 1/2)</td>
<td>Fm3m'</td>
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<td>35</td>
<td>(3^* x-1/2, x+1/2, x; -1/2, 1/2, 0)</td>
<td>Fm3m'</td>
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<td>36</td>
<td>(3^* x+1/2, x+1/2, x; 1/2, 1/2, 0)</td>
<td>Fm3m'</td>
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<td>37</td>
<td>(g^* (-1/4, 1/4, 1/2) x+1/4, \overline{x}, z)</td>
<td>Fm3m'</td>
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<tr>
<td>38</td>
<td>(g^* (1/4, 1/4, 1/2) x-1/4, x, z)</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>39</td>
<td>(4^* -1/4, 1/4, z; -1/4, 1/4, 1/4 (4^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>40</td>
<td>(4^* 1/4, 1/4, z; 1/4, 1/4, 1/4 (4^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>41</td>
<td>(4^* x, 0, 1/2; 0, 0, 1/2 (4^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>42</td>
<td>(m^* x, y+1/2, y (m^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>43</td>
<td>(g^* (0, 1/2, 1/2) x, y, y (m^* y, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>44</td>
<td>(4^* x, 1/2, 0; 0, 1/2, 0 )</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>45</td>
<td>(4^* -1/4, y, 1/4; -1/4, 1/4, 1/4 (4^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td></td>
<td>(g^* (1/4, 1/2, 1/4) x+1/4, y, x )</td>
<td>Fm3m'</td>
</tr>
<tr>
<td></td>
<td>((4^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
</tbody>
</table>

For \((1/2, 0, 1/2)\) set:

<table>
<thead>
<tr>
<th>Set</th>
<th>Formula</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>46</td>
<td>(2 (1/2, 0, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>47</td>
<td>(4^* 1/4, y, 1/4; 1/4, 1/4, 1/4 (4^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
<tr>
<td>48</td>
<td>(g^* (1/4, 1/2, 1/4) x-1/4, y, x )</td>
<td>Fm3m'</td>
</tr>
<tr>
<td></td>
<td>((m^* x, 0, 1/2, 1/2))</td>
<td>Fm3m'</td>
</tr>
</tbody>
</table>

Continued 225.4.1621 Fm3m'
Continued
225.4.1621 Fm3m'

(1) t (1/2,1/2,0) + set
(1) 1/2,1/2,0)
(2) 2 1/4,1/4,z
(2) 1/2,1/2,0)
(3) 2 0,1/2,0) 1/4,y,0
(3) 1/2,1/2,0) x,1/4,0
(4) 2 1/2,0,0) + x,1/4,0
(4) 1/2,1/2,0) + x,1/4,0
(5) 3+ (1/3,1/3,1/3)
(5) 3+ x+1/2,x,x
(6) 3+ x+1/2,x,x
(7) 3+ x+1/2,x,x
(8) 3+ (1/3,1/3,-1/3)
(9) 3+ (1/3,1/3,-1/3)
(10) 3+ x,x+1/2,x
(11) 3+ x,x+1/2,x
(12) 3+ x,x+1/2,x
(13) 2' (1/2,1/2,0) + x,x,0
(14) 2' x,x+1/2,0
(15) 4+ * 1/2,0,z
(16) 4+ * 0,1/2,z
(17) 4+ ' (1/2,0,0) + x,1/4,-1/4
(18) 2' (0,1/4,1/4) 1,4,y+1/4,y
(19) 2' (0,1/4,-1/4) 1,4,y+1/4,y
(20) 4+ ' (1/2,0,0) + x,1/4,1/4
(21) 4+ ' (0,1/2,0) + 1,4,y,-1/4
(22) 2' (1/4,0,1/4) x+1/4,1/4,x
(23) 4+ ' (0,1/2,0) + 1,4,y,1/4
(24) 2' (1/4,0,-1/4) x+1/4,1/4,x
(25) 1/4,1/4,0
(26) n 1/2,1/2,0)
(27) a (1/2,0,0) + x,1/4,0
(28) b (0,1/2,0) + 1/4,y,z
(29) 3+ x+1/2,x,x;
(30) 3+ x+1/2,x,x;
(31) 3+ x+1/2,x,x;
(32) 3+ x+1/2,x,x;
(33) 3+ x+1/2,x,x;
(34) 3+ x+1/2,x,x;
(35) 3+ x+1/2,x,x;
(36) 3+ x+1/2,x,x;
(37) m' x+1/2,x,z
(38) g' (1/2,1/2,0) x,x,z
(39) 4+ * 0,1/2,z; 0,1/2,0
(40) 4+ * 0,1/2,z; 0,1/2,0
(41) 4+ ' x,1/4,1/4; 1/4,1/4,1/4
(42) g' (1/2,1/4,-1/4) x,y+1/4,y
(43) g' (1/2,1/4,1/4) x,y+1/4,y
(44) 4+ ' x,1/4,-1/4; 1/4,1/4,-1/4
(45) 4+ ' x,1/4,-1/4; 1/4,1/4,-1/4
(46) g' (1/4,1/2,-1/4) x+1/4,y,x
(47) 4+ ' 1/4,y,-1/4; 1/4,1/4,-1/4
(48) g' (1/4,1/2,1/4) x+1/4,y,x

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

192 1 1

(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) x,y,z [u,v,w]
(4) x,y,z [u,v,w]
(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]

Coordinates

(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
48  g  2.m'm'  x,1/4,1/4 [u,0,0]  \bar{x},3/4,1/4 [\bar{u},0,0]  1/4,\bar{x},1/4 [0,\bar{u},0]  1/4,\bar{x},3/4 [0,\bar{u},0]

1/4,1/4,x [0,0,u]  3/4,1/4,\bar{x} [0,0,\bar{u}]  1/4,\bar{x},3/4 [0,\bar{u},0]  3/4,\bar{x},3/4 [0,\bar{u},0]

x,1/4,3/4 [\bar{u},0,0]  \bar{x},1/4,1/4 [u,0,0]  1/4,1/4,\bar{x} [0,0,u]  1/4,3/4,x [0,0,u]

32  f  .3m'  x,x,x [u,u,u]  \bar{x},\bar{x},x [\bar{u},\bar{u},u]  \bar{x},x,x [u,\bar{u},u]  \bar{x},x,x [u,\bar{u},u]

x,x,\bar{x} [\bar{u},\bar{u},\bar{u}]  \bar{x},x,\bar{x} [\bar{u},\bar{u},\bar{u}]  x,x,\bar{x} [u,u,\bar{u}]  \bar{x},\bar{x},x [u,\bar{u},\bar{u}]

24  e  4'm.m'  x,0,0 [0,0,0]  \bar{x},0,0 [0,0,0]  0,x,0 [0,0,0]

0,\bar{x},0 [0,0,0]  0,0,x [0,0,0]  0,\bar{x},0 [0,0,0]

24  d  m.m'm'  0,1/4,1/4 [u,0,0]  0,3/4,1/4 [\bar{u},0,0]  1/4,0,1/4 [0,u,0]

1/4,0,3/4 [0,\bar{u},0]  1/4,1/4,0 [0,0,u]  3/4,1/4,0 [0,0,\bar{u}]

8   c  4'3m'  1/4,1/4,1/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]

4   b  m3m'  1/2,1/2,1/2 [0,0,0]

4   a  m\bar{3}m'  0,0,0 [0,0,0]

Symmetry of Special Projections

Along [0,0,1]   p4mm1'  Along [1,1,1]   p6'mm'  Along [1,1,0]   c2'mm'
\text{s}{\text{a}^*} = a/2   \text{s}{\text{b}^*} = b/2  \text{s}{\text{a}^*} = (2a - b - c)/6   \text{s}{\text{b}^*} = (-a + 2b - c)/6  \text{s}{\text{a}^*} = c   \text{s}{\text{b}^*} = (-a + b)/2

Origin at 0,0,z  Origin at x,x,x  Origin at x,x,0
Origin at center (m’3’m’)

Asymmetric unit

\[ 0 \leq x \leq \frac{1}{2}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq \frac{1}{4}; \quad y \leq \min(x, \frac{1}{2} - x); \quad z \leq y \]

Vertices

\[(0,0,0) \quad \frac{1}{2},0,0 \quad \frac{1}{4},\frac{1}{4},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 \quad 0,0,z \\
(3) & \quad 2 \quad y,0,0 \\
(4) & \quad 2 \quad x,0,0 \\
(5) & \quad 3^+ \quad x,x,x \\
(6) & \quad 3^+ \quad x,x,x \\
(7) & \quad 3+ \quad x,x,x \\
(8) & \quad 3^+ \quad x,x,x \\
(9) & \quad 3^- \quad x,x,x \\
(10) & \quad 3^- \quad x,x,x \\
(11) & \quad 3^- \quad x,x,x \\
(12) & \quad 3^- \quad x,x,x
\end{align*}
\]

\[
\begin{align*}
(1) & \quad 1 \\
(2) & \quad 0,0,0 \\
(3) & \quad 0,0,0 \\
(4) & \quad 0,0,0 \\
(5) & \quad 0,0,0 \\
(6) & \quad 0,0,0 \\
(7) & \quad 0,0,0 \\
(8) & \quad 0,0,0 \\
(9) & \quad 0,0,0 \\
(10) & \quad 0,0,0 \\
(11) & \quad 0,0,0 \\
(12) & \quad 0,0,0
\end{align*}
\]
Continued

225.5.1622

Fm'3m'

(13) 2 x,x,0
(2,xy | 0,0,0)
(14) 2 x,x,0
(2,xy | 0,0,0)
(15) 4' 0,0,0
(4, | 0,0,0)
(16) 4' 0,0,0
(4, | 0,0,0)
(17) 4' x,0,0
(4,x | 0,0,0)
(18) 2 0,y,y
(2,yz | 0,0,0)
(19) 2 0,y,y
(2,yz | 0,0,0)
(20) 4' x,0,0
(4, | 0,0,0)
(21) 4' 0,y,0
(4,y | 0,0,0)
(22) 2 x,0,x
(2,xz | 0,0,0)
(23) 4' 0,y,0
(4, | 0,0,0)
(24) 2 x,0,x
(2,xz | 0,0,0)
(25) 1' 0,0,0
(1 | 0,0,0)
(26) m' x,y,0
(m,xy | 0,0,0)
(27) m' x,0,z
(m,xy | 0,0,0)
(28) m' 0,y,z
(m,xy | 0,0,0)
(29) 3' x,x,x; 0,0,0
(3,xyz | 0,0,0)
(31) 3' x,x,x; 0,0,0
(3,xyz | 0,0,0)
(32) 3' x,x,x; 0,0,0
(3,xyz | 0,0,0)
(33) 3' x,x,x; 0,0,0
(3,xyz | 0,0,0)
(34) 3' x,x,x; 0,0,0
(3,xyz | 0,0,0)
(36) 3' x,x,x; 0,0,0
(3,xyz | 0,0,0)
(37) m' x,x,z
(m,xyz | 0,0,0)
(38) m' x,x,z
(m,xyz | 0,0,0)
(39) 4' 0,0,z; 0,0,0
(4, | 0,0,0)
(40) 4' 0,0,z; 0,0,0
(4, | 0,0,0)
(41) 4' x,0,0; 0,0,0
(4,x | 0,0,0)
(42) m' x,y,y
(m,xy | 0,0,0)
(43) m' x,y,y
(m,xy | 0,0,0)
(44) 4' x,0,0; 0,0,0
(4,x | 0,0,0)
(45) 4' 0,y,0; 0,0,0
(4,y | 0,0,0)
(46) m' x,y,x
(m,xyz | 0,0,0)
(47) 4' 0,y,0; 0,0,0
(4, | 0,0,0)
(48) m' x,y,x
(m,xyz | 0,0,0)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)
(2) t (0,1/2,1/2)
(3) 2 (0,1/2,0) 0,1/4,z
(2,y | 0,1/2,1/2)
(4) 2 x,1/4,1/4
(2,z | 0,1/2,1/2)
(5) 3' (1/3,1/3,1/3)
(3,xyz | 0,1/2,1/2)
(6) 3' x,x+1/2,x
(3,xyz | 0,1/2,1/2)
(7) 3' (-1/3,1/3,1/3)
(3,xyz | 0,1/2,1/2)
(8) 3' x,x+1/2,x
(3,xyz | 0,1/2,1/2)
(9) 3' (1/3,1/3,1/3)
(3,xyz | 0,1/2,1/2)
(10) 3' (-1/3,1/3,1/3)
(3,xyz | 0,1/2,1/2)
(11) 3' x,x+1/2,x+1/2,x
(3,xyz | 0,1/2,1/2)
(12) 3' x,x+1/2,x+1/2,x
(3,xyz | 0,1/2,1/2)
(13) 2 (1/4,1/4,0)
(2,xy | 0,1/2,1/2)
(14) 2 (-1/4,1/4,0)
(2,xy | 0,1/2,1/2)
(15) 4' (0,0,1/2) 1/4,1/4,z
(4, | 0,1/2,1/2)
(16) 4' (0,0,1/2) -1/4,1/4,z
(4, | 0,1/2,1/2)
(17) 4' x,1/2,0
(4,x | 0,1/2,1/2)
(18) 2 (0,1/2,1/2)
(2,z | 0,1/2,1/2)
(19) 2 0,y+1/2,y
(2,yz | 0,1/2,1/2)
(20) 4' x,0,1/2
(4,z | 0,1/2,1/2)
(21) 4' (0,1/2,0) 1/4,y,1/4
(4,y | 0,1/2,1/2)
(22) 2 (1/4,0,1/4)
(2,yz | 0,1/2,1/2)
(23) 4' (0,1/2,0) -1/4,y,1/4
(4, | 0,1/2,1/2)
(24) 2 (-1/4,0,1/4)x,x+1/4,1/4,x
(2,xz | 0,1/2,1/2)
(25) 1' 0,1/4,1/4
(1 | 0,1/2,1/2)
(26) b' (0,1/2,0)
(2,yz | 0,1/2,1/2)
(27) c' (0,0,1/2)
(2,yz | 0,1/2,1/2)
(28) n' (0,1/2,1/2)
(2,yz | 0,1/2,1/2)
(29) 3' x,x+1/2,x;
0,1/2,0
(3,xyz | 0,1/2,1/2)
(30) 3' x,x+1/2,x;
0,1/2,0
(3,xyz | 0,1/2,1/2)
Continued

(33) $\tilde{\mathbf{3}}^* \cdot x-1/2,x-1/2,x; \quad 0,0,1/2$

(34) $\tilde{\mathbf{3}}^* \cdot x+1/2,x-1/2,x; \quad 0,0,1/2$

(35) $\tilde{\mathbf{3}}^* \cdot x-1/2,x+1/2,x; \quad 1/2,1/2,0$

(36) $\tilde{\mathbf{3}}^* \cdot x+1/2,x+1/2,x; \quad 1/2,1/2,0$

(37) $g'$ (-1/4,1/4,1/4) \quad x+1/4,\bar{x},z \quad (m_yz) [0,1/2,1/2]'

(38) $g' (1/4,1/4,1/4) \quad x-1/4,x,z \quad (m_yz) [0,1/2,1/2]'

(39) $\tilde{\mathbf{4}} \cdot -1/4,1/4,4,4,1/4 \quad z; 1/4,1/4,1/4 \quad (\bar{z}) [0,1/2,1/2]'$

(40) $\tilde{\mathbf{4}} \cdot 1/4,1/4,4,1/4 \quad z; 1/4,1/4,1/4 \quad (\bar{z}) [0,1/2,1/2]'$

(41) $\tilde{\mathbf{4}} \cdot x,0,1/2; 0,0,1/2$

(42) $\tilde{\mathbf{4}} \cdot x,y+1/2,y$

(43) $g' (0,1/2,1/2) \quad x,0,1/2$

(44) $\tilde{\mathbf{4}} \cdot x,1/2,0; 0,1/2,0$

(45) $\tilde{\mathbf{4}} \cdot -1/4,y,1/4,-1/4,1/4,1/4$

For (1/2,0,1/2) + set

(1) t (1/2,0,1/2)

(2) 2 (0,0,1/2) \quad 1/4,0,z

(3) 2 \quad 1/4,y+1/4

(4) 2 (1/2,0,0) \quad x,0,1/2

(5) 3' (1/3,1/3,1/3)

(6) 3' (1/3,-1/3,1/3)

(7) 3' \quad x+1/2, x-1/2, x

(8) 3' \quad x+1/2, x+1/2, x

(9) 3 (1/3,1/3,1/3)

(10) 3' \quad x+1/2, x+1/2, x

(11) 3' \quad x+1/2, x+1/2, x

(12) 3 (1/3,-1/3,1/3)

(13) 2 (1/4,1/4,0) \quad x,x-1/4,1/4

(14) 2 (1/4,-1,1/4) \quad x,x+1/4,1/4

(15) 4' (0,0,1/2) \quad 1/4,-1,4/4,1/4

(16) 4' (0,0,1/2) \quad 1/4,-1,4/4,1/4

(17) 2 (1/2,0,1/2)

(18) 2 (0,1/4,1/4) \quad x,x-1/6,1/2

(19) 2 (0,-1,2,1/2) \quad x,x+1/4,1/4

(20) 4' (1/2,0,0) \quad x,x-1/4,1/4

(21) 4' \quad 1/2,y,0

(22) 2 (1/2,0,1/2) \quad x,y,x

(23) 4' \quad 0,y,1/2

(24) 2 \quad x+1/2,0,x

(25) 2 \quad 0,y,1/2

(26) 2 (1/2,0,1/2) \quad x,y+1/2, x+1/2, x

(27) n' (1/2,0,1/2) \quad x,y+1/2, x+1/2, x

(28) c' (0,0,1/2) \quad 1/4,y, z

(29) 3' \cdot x-1/2,x-1/2,x; \quad 0,0,1/2

(30) 3' \cdot x-1/2,x+1/2,x; \quad 0,0,1/2

(31) 3' \cdot x+1/2,x+1/2,x; \quad 0,0,1/2

(32) 3' \cdot x+1/2,x-1/2,x; \quad 0,0,1/2

(33) 3' \cdot x+1/2,x; \quad 1/2,0,0

(34) 3' \cdot x+1/2,x, x; \quad 1/2,0,0

(35) 3' \cdot x+1/2,x, x; \quad 1/2,0,0

(36) 3' \cdot x+1/2,x, x; \quad 1/2,0,0

(37) g' (1/4,-1,1/4,1/4) \quad x+1/4,\bar{x},z

(38) g' (1/4,1/4,1/4,1/4) \quad x+1/4,x,z

(39) 4' \cdot 1/4,1/4,1/4 \quad z; 1/4,1/4,1/4

(40) 4' \cdot 1/4,1/4,1/4 \quad z; 1/4,1/4,1/4

(41) \tilde{\mathbf{4}} \cdot x,-1/4,1/4,1/4 \quad x,y+1/4,1/4,1/4

(42) g' (1/2,-1,4,1/4) \quad x,y-1/4,1/4,1/4

(43) g' (1/2,1/2,1/2) \quad x,y+1/4,1/4,1/4

(44) g' (1/2,1/2,1/2) \quad x,y+1/4,1/4,1/4

(45) \tilde{\mathbf{4}} \cdot x,0,1/2; 0,0,1/2

(46) \tilde{\mathbf{4}} \cdot x,0,1/2; 0,0,1/2

(47) 4' \cdot 1/2,y,0; 1/2,0,0

(48) 4' \cdot 1/2,y,0; 1/2,0,0
Continued

225.5.1622  Fm'3'm'

For (1/2,1/2,0) + set

\begin{align*}
(1) & \ t(1/2,1/2,0) \\
(2) & \ t(1/2,1/2,0) \\
(3) & \ t(1/2,1/2,0) \\
(4) & \ t(1/2,1/2,0) \\
(5) & \ t(1/3,1/3,1/3) \\
(6) & \ t(1/2,1/2,0) \\
(7) & \ t(1/2,1/2,0) \\
(8) & \ t(1/2,1/2,0) \\
(9) & \ x+1/2,x,x+1/2 \\
(10) & \ x+1/2,x,x+1/2 \\
(11) & \ x+1/2,x,x+1/2 \\
(12) & \ x+1/2,x,x+1/2 \\
(13) & \ x+1/2,x,x+1/2 \\
(14) & \ x+1/2,x,x+1/2 \\
(15) & \ x+1/2,x,x+1/2 \\
(16) & \ x+1/2,x,x+1/2 \\
(17) & \ x+1/2,x,x+1/2 \\
(18) & \ x+1/2,x,x+1/2 \\
(19) & \ x+1/2,x,x+1/2 \\
(20) & \ x+1/2,x,x+1/2 \\
(21) & \ x+1/2,x,x+1/2 \\
(22) & \ x+1/2,x,x+1/2 \\
(23) & \ x+1/2,x,x+1/2 \\
(24) & \ x+1/2,x,x+1/2 \\
(25) & \ x+1/2,x,x+1/2 \\
(26) & \ x+1/2,x,x+1/2 \\
(27) & \ x+1/2,x,x+1/2 \\
(28) & \ x+1/2,x,x+1/2 \\
(29) & \ x+1/2,x,x+1/2 \\
(30) & \ x+1/2,x,x+1/2 \\
(31) & \ x+1/2,x,x+1/2 \\
(32) & \ x+1/2,x,x+1/2 \\
(33) & \ x+1/2,x,x+1/2 \\
(34) & \ x+1/2,x,x+1/2 \\
(35) & \ x+1/2,x,x+1/2 \\
(36) & \ x+1/2,x,x+1/2 \\
(37) & \ x+1/2,x,x+1/2 \\
(38) & \ x+1/2,x,x+1/2 \\
(39) & \ x+1/2,x,x+1/2 \\
(40) & \ x+1/2,x,x+1/2 \\
(41) & \ x+1/2,x,x+1/2 \\
(42) & \ x+1/2,x,x+1/2 \\
(43) & \ x+1/2,x,x+1/2 \\
(44) & \ x+1/2,x,x+1/2 \\
(45) & \ x+1/2,x,x+1/2 \\
(46) & \ x+1/2,x,x+1/2 \\
(47) & \ x+1/2,x,x+1/2 \\
(48) & \ x+1/2,x,x+1/2 \\
\end{align*}

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity
Wyckoff letter,
Site Symmetry.

192  l  1

(1) x,y,z [u,v,w]  
(2) x,y,z [u,v,w]  
(3) x,y,z [u,v,w]  
(4) x,y,z [u,v,w]  
(5) z,x,y [w,u,v]  
(6) z,x,y [w,u,v]  
(7) z,x,y [w,u,v]  
(8) z,x,y [w,u,v]  

\begin{align*}
\text{Coordinates} \\
(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
\end{align*}
48  g  2.m'm'  x,1/4,1/4 [u,0,0]  x,3/4,1/4 [u,0,0]  1/4,x,1/4 [0,u,0]  1/4,x,3/4 [0,u,0]  
1/4,1/4,x [0,0,u]  3/4,1/4,x [0,0,u]  1/4,x,3/4 [0,u,0]  3/4,x,3/4 [0,u,0]  
x,1/4,3/4 [u,0,0]  x,1/4,1/4 [u,0,0]  1/4,1/4,x [0,0,u]  1/4,3/4,x [0,0,u]  
32  f  .3m'  x,x,x [u,u,u]  x,x,x [u,u,u]  x,x,x [u,u,u]  x,x,x [u,u,u]  
24  e  4m'.m'  x,0,0 [u,0,0]  x,0,0 [u,0,0]  0,x,0 [0,u,0]  0,x,0 [0,u,0]  
0,x,0 [0,u,0]  0,0,x [0,u,0]  0,0,x [0,u,0]  
24  d  m'.m'm'  0,1/4,1/4 [0,0,0]  0,3/4,1/4 [0,0,0]  1/4,0,1/4 [0,0,0]  1/4,0,1/4 [0,0,0]  
1/4,0,3/4 [0,0,0]  1/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]  3/4,1/4,0 [0,0,0]  
8   c  43'm'  1/4,1/4,1/4 [0,0,0]  1/4,1/4,3/4 [0,0,0]  
4   b  m33'm'  1/2,1/2,1/2 [0,0,0]  
4   a  m3m'  0,0,0 [0,0,0]  

Symmetry of Special Projections

Along [0,0,1] p4m'm'  
\[a^* = a/2 \quad b^* = b/2\]  
Origin at 0,0,z

Along [1,1,1] p6m'm'  
\[a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6\]  
Origin at x,x,x

Along [1,1,0] c2m'm'  
\[a^* = (-a + b)/2 \quad b^* = c\]  
Origin at x,x,0
Origin at center ($m\overline{3}$)

Asymmetric unit

\begin{align*}
0 \leq x & \leq 1/2; & 0 \leq y & \leq 1/4; & 0 \leq z & \leq 1/4; & y \leq \min(x, 1/2-x); & z \leq y
\end{align*}

Vertices

\begin{align*}
0,0,0 & & 1/2,0,0 & & 1/4,1/4,0 & & 1/4,1/4,1/4
\end{align*}

Symmetry Operations

For \((0,0,0) + \text{ set}\)

\begin{align*}
(1) & & 1 & & (2) & & 2 \ 0,0,z & & (3) & & 2 \ 0,y,0 & & (4) & & 2 \ x,0,0 & \\
(1) & & (0,0,0) & & (2) & & \ (2z,0,0,0) & & (3) & & \ (2y,0,0,0) & & (4) & & \ (2x,0,0,0) \\
(5) & & 3^{+} \ x,z,\bar{x} & & (6) & & 3^{+} \ x,\bar{x},x & & (7) & & 3^{+} \ x,\bar{x},x & & (8) & & 3^{+} \ x,\bar{x},x \\
(3_{xyz}|0,0,0) & & (3_{xyz}|1,0,0) & & (3_{xyz}|1,0,0) & & (3_{xyz}|0,0,0) & & (3_{xyz}|0,0,0) & & (3_{xyz}$^{-1}$|0,0,0) \\
(9) & & 3^{+} \ x,\bar{x},x & & (10) & & 3^{+} \ x,\bar{x},x & & (11) & & 3^{+} \ x,\bar{x},x & & (12) & & 3^{+} \ x,\bar{x},x \\
(3_{xyz}|0,0,0) & & (3_{xyz}|0,0,0) & & (3_{xyz}|0,0,0) & & (3_{xyz}|0,0,0) & & (3_{xyz}$^{-1}$|0,0,0) & & (3_{xyz}$^{-1}$|0,0,0)
\end{align*}
Continued

(33) $3^+ \ x-1/2,x-1/2,x$; $0,0,1/2$

(34) $3^+ x+1/2,x-1/2,x$; $0,0,1/2$

(35) $3^+ x-1/2,x+1/2,x$; $-1/2,1/2,0$

(36) $3^+ x+1/2,x+1/2,x$; $1/2,1/2,0$

(37) $g (1/4,-1/4,0)$ $x+1/4,x,z$

(38) $g (1/4,1/4,0)$ $x+1/4,x,z$

(39) $4^+ 1/4,1/4,z; 1/4,1/4,0$

(40) $4^+ 1/4,-1/4,z; 1/4,-1/4,0$

(41) $4^+ x,0,0; 1/4,0,0$

(42) $a (1/2,0,0)$ $x,y,\bar{y}$

(43) $a (1/2,0,0)$ $x,y,y$

(44) $4^+ x,0,0; 1/4,0,0$

(45) $4^+ 1/4,y,1/4; 1/4,0,1/4$

(46) $g (1/4,0,-1/4) x+1/4,y,x$

(47) $4^+ 1/4,y,-1/4; 1/4,0,-1/4$

(48) $g (1/4,0,1/4) x+1/4,y,x$

For $(1/2,0,1/2) +$ set

(1) $t (1/2,0,1/2)$

(2) $2 (0,0,1/2) 1/4,0,z$

(3) $2 1/4,y,1/4$

(4) $2 (1/2,0,0) x,0,1/4$

(5) $3^+ (1/3,1/3,1/3)$ $x+1/6,x-1/6,x$

(6) $3^+ (1/3,-1/3,1/3)$ $x+1/6,x+1/6,x$

(9) $3^+ (1/3,1/3,1/3)$ $x-1/6,x+1/3,x$

(10) $3^+ x+1/2,x,\bar{x}$

(11) $3^+ x+1/2,\bar{x},x$

(12) $3^+ (1/3,-1/3,1/3)$ $x-1/6,x+1/3,x$

(13) $2 (1/4,1/4,0)$ $x,x+1/4,0$

(14) $2 (-1/4,1/4,0) x,x+1/4,0$

(15) $4^+ 1/4,1/4,z$

(16) $4^+ -1/4,1/4,z$

(17) $4^+ x,1/4,-1/4$

(18) $2 (0,1/4,1/4) 0,y+1/4,y$

(19) $2 (0,1/4,-1/4) 0,y+1/4,y$

(20) $4^+ -1/4,1/4,z$

(21) $4^+ (0,1/2,0) 0,y,0$

(22) $2 x,1/4,x$

(23) $4^+ (0,1/2,0) 0,y,0$

(24) $2 1/4,x$

(25) $\bar{1} 1/4,0,1/4$

(1) $1/2,0,1/2$

(26) $a (1/2,0,0) x,y,1/4$

(27) $n (1/2,0,1/2) x,0,z$

(28) $c (0,0,1/2) 1/4,y,z$

(29) $3^+ x-1/2,x+1/2,x$; $0,0,1/2$

(30) $3^+ x-1/2,x+1/2,x$; $0,0,1/2$

(31) $3^+ x+1/2,\bar{x}+1/2,x$; $1/2,1/2,0$

(32) $3^+ x+1/2,\bar{x}-1/2,x$; $1/2,-1/2,0$

(33) $3^+ x+1/2,x,x$; $1/2,0,0$

(34) $3^+ x+1/2,x,-1,x$; $1/2,0,0$

(35) $3^+ x+1/2,x+1,x$; $0,1/2,1/2$

(36) $3^+ x+1/2,x,x$; $0,1/2,1/2$

(37) $g (-1/4,1/4,0)$ $x+1/4,x,z$

(38) $g (1/4,1/4,0) x-1/4,x,z$

(39) $4^+ -1/4,1/4,z; -1/4,1/4,0$

(40) $4^+ 1/4,1/4,z; 1/4,1/4,0$

(41) $4^+ x,1/4,1/4; 0,1/4,1/4$

(42) $g (0,1/4,-1/4) x,y+1/4,y$

(43) $g (0,1/4,1/4) x,y+1/4,y$

(44) $4^+ x,1/4,-1/4; 0,1/4,-1/4$

(45) $4^+ 0,y,0; 0,1/4,0$

(46) $b (0,1/2,0) \bar{x},y,x$

(47) $4^+ 0,y,0; 0,1/4,0$

(48) $b (0,1/2,0) x,y,x$

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Continued 226.1.1623 Fm3c

For (1/2,1/2,0) + set

<table>
<thead>
<tr>
<th>No.</th>
<th>Description</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>t (1/2,1/2,0)</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0)</td>
</tr>
<tr>
<td>2</td>
<td>2 1/4,1/4, z</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>(2z1/2,1/2,0)</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>2 (0,1/2,0) 1/4,y,0</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>(2z1/2,1/2,0)</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>3+ x+1/2,x, x</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>3+ x+1/2,x, x</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>3+ (1/3,1/3,1/3) x+1/6,x+1/3,x</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>3+ (1/3,1/3,1/3) x+1/3,x+1/6,x</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>3- x,x+1/2,x</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>3+ (1/3,1/3,1/3) x+1/3,x+1/6,x</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>3- x,x+1/2,x</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>2 x,x,1/4</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>2 x,x,1/4</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>4+ (0,0,1/2) 0,0,z</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>4+ (0,0,1/2) 0,0,z</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>4+ x,1/4,1/4</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>4+ (0,1/4,1/4) 0,y-1/4,y</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>4+ (0,1/4,1/4) 0,y+1/4,y</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>4+ x,-1/4,1/4</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>4+ 1/4,y,1/4</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>2 (1/4,0,1/4) x-1/4,0,x</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>4+ -1/4,y,1/4</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>2 (-1/4,0,1/4) x-1/4,0,x</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>(1/2,1/2,0)</td>
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</tr>
<tr>
<td>26</td>
<td>n (1/2,1/2,0) x,y,0</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>a (1/2,0,0) 1/4,y,z</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>b (0,1/2,0) 1/4,y,z</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>3+ x+1/2,x,x; 1/2,0</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>3+ x+1/2,x,x; 1/2,0</td>
<td></td>
</tr>
<tr>
<td>31</td>
<td>3+ x+1/2,x,x+1/2,x; 1/2,0</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>3+ x+1/2,x,x; 1/2,0</td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>3- x+1/2,x; 0,1/2</td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>3- x+1/2,x; 0,1/2</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>3- x+1/2,x; 0,1/2</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>3- x+1,1/2,x, 1/2,x</td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>c (0,0,1/2) x,x,z</td>
<td></td>
</tr>
<tr>
<td>38</td>
<td>c (0,0,1/2) x,x,z</td>
<td></td>
</tr>
<tr>
<td>39</td>
<td>4+ 0,0,z; 0,0,1/4</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>4+ 0,0,z; 0,0,1/4</td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>4- x,-1/4,1/4, 0,-1/4,1/4</td>
<td></td>
</tr>
<tr>
<td>42</td>
<td>g (0,-1/4,1/4) x,y+1/4,y</td>
<td></td>
</tr>
<tr>
<td>43</td>
<td>g (0,1/4,1/4) x,y-1/4,y</td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>4+ x,1/4,1/4; 0,1/4,1/4</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>4+ x,-1/4,1/4; 0,-1/4,0,1/4</td>
<td></td>
</tr>
<tr>
<td>46</td>
<td>g (-1/4,1/4,0) x+1/4,y,x</td>
<td></td>
</tr>
</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).
### Symmetry of Special Projections

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
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<tr>
<td>Symmetry of Special Projections</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Along $[0,0,1]$  
**p4mm1'**  
$a^* = a/2$  
$b^* = b/2$  
Origin at 0,0,z

Along $[1,1,1]$  
**p6'm'm**  
$a^* = (2a - b - c)/6$  
$b^* = (-a + 2b - c)/6$  
Origin at x,x,x

Along $[1,1,0]$  
**p2mm1'**  
$a^* = (-a + b)/4$  
$b^* = c/2$  
Origin at x,x,0
Origin at center \((m\overline{3}1')\)

Asymmetric unit: \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad z \leq y\)

Vertices: \((0,0,0)\), \((1/2,0,0)\), \((1/4,1/4,0)\), \((1/4,1/4,1/4)\)

Symmetry Operations:

For \((0,0,0)\) + set:

1. \((1) \bar{1}\)
2. \((2) \bar{0},0,z\)
3. \((3) \bar{2},0,y,0\)
4. \((4) \bar{2},x,0,0\)
5. \((5) \bar{3}^+ x,x,x\)
6. \((6) \bar{3}^- x,x,x\)
7. \((7) \bar{3}^+ x,x,x\)
8. \((8) \bar{3}^- x,x,x\)
9. \((9) 3^- x,x,x\)
10. \((10) 3^+ x,x,x\)
11. \((11) 3^- x,x,x\)
12. \((12) 3^+ x,x,x\)

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Continued

(13) 2 (1/2,1/2,0) x,x,1/4
(2_{xy}|1/2,1/2,1/2)

(14) 2 x,x+1/2,1/4
(2_{xy}|1/2,1/2,1/2)

(15) 4' (0,0,1/2) 1/2,0,z
(4_{z}^{-1}|1/2,1/2,1/2)

(16) 4' (0,0,1/2) 0,1/2,z
(4_{z}|1/2,1/2,1/2)

(17) 4' (1/2,0,0) x,1/2,0
(4_{xy}^{-1}|1/2,1/2,1/2)

(18) 2 (0,1/2,1/2) 1/4,y,y
(2_{y}|1/2,1/2,1/2)

(19) 2 1/4,y+1/2,y
(2_{y}|1/2,1/2,1/2)

(20) 4' (1/2,0,0) x,0,1/2
(4_{x}|1/2,1/2,1/2)

(21) 4' (0,1/2,0) 1/2,y,0
(4_{y}|1/2,1/2,1/2)

(22) 2 (1/2,0,1/2) x,1/4,x
(2_{xz}|1/2,1/2,1/2)

(23) 4' (0,1/2,0) 0,y,1/2
(4_{y}^{-1}|1/2,1/2,1/2)

(24) 2 x+1/2,1/4,x
(2_{xz}|1/2,1/2,1/2)

(25) 1 0,0,0
(1|0,0,0)

(26) m x,y,0
(m_{y}|0,0,0)

(27) m x,0,z
(m_{y}|0,0,0)

(28) m 0,y,z
(m_{x}|0,0,0)

(29) 3^+ x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(30) 3^+ x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(31) 3^+ x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(32) 3^+ x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(33) 3^+ x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(34) 3^- x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(35) 3^- x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(36) 3^- x,x,x; 0,0,0
(3_{xy}^{-1}|0,0,0)

(37) c (0,0,1/2) x+1/2,x,z
(m_{y}|1/2,1/2,1/2)

(38) n (1/2,1/2,1/2) x,x,z
(m_{y}|1/2,1/2,1/2)

(39) 4' 0,1/2,z; 0,1/2,1/4
(4_{z}^{-1}|1/2,1/2,1/2)

(40) 4^+ 1/2,0,z; 1/2,0,1/4
(4_{x}|1/2,1/2,1/2)

(41) 4^- x,0,1/2; 1/4,0,1/2
(4_{xy}^{-1}|1/2,1/2,1/2)

(42) a (1,0,2,0) x,y+1/2,y
(m_{y}|1/2,2,1,1/2)

(43) n (1/2,1/2,1/2) x,y,y
(m_{y}|1/2,2,1,1/2)

(44) 4^- x,1/2,0; 1/4,1,2,0
(4_{x}|1/2,1/2,1/2)

(45) 4^- 0,1/2,0; 1/4,1,2,0
(4_{xy}|1/2,1/2,1/2)

(46) b (0,1/2,0) x+1/2,y,x
(m_{yz}|1/2,1/2,1/2)

(47) 4^- 1/2,y,0; 1/2,1/4,0
(4_{y}^{-1}|1/2,1/2,1/2)

(48) n (1/2,1/2,1/2) x,y,x
(m_{yz}|1/2,1/2,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)
(1 0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z
(2_{z}|0,1/2,1/2)

(3) 2 (0,1/2,0) 0,y,1/4
(2_{y}|0,1/2,1/2)

(4) 2 x,1/4,1/4
(2_{z}|0,1/2,1/2)

(5) 3^+ (1/3,1/3,1/3)
(3_{xy}^{-1}|0,1/2,1/2)

(6) 3^- x,x+1/2,x
(3_{xy}^{-1}|0,1/2,1/2)

(7) 3^- (-1/3,1/3,1/3)
(3_{xy}^{-1}|0,1/2,1/2)

(8) 3^- x,x+1/2,x
(3_{xy}^{-1}|0,1/2,1/2)

(9) 3^- (-1/3,1/3,1/3)
(3_{xy}^{-1}|0,1/2,1/2)

(10) 3^- x,x+1/2,x+1/2,x
(3_{xy}^{-1}|0,1/2,1/2)

(11) 3^- x,x+1/2,x+1/2,x
(3_{xy}^{-1}|0,1/2,1/2)

(12) 3^- x,-1/2,x+1/2,x
(3_{xy}^{-1}|0,1/2,1/2)

(13) 2 (1/4,1/4,0)
(2_{xy}^{-1}|1/2,0,0)

(14) 2 (1/4,-1/4,0) x,x+1/4,0
(2_{xy}^{-1}|1/2,0,0)

(15) 4^- 1/4,-1/4,z
(4_{z}^{-1}|1/2,0,0)

(16) 4^- 1/4,1/4,z
(4_{z}^{-1}|1/2,0,0)

(17) 4^- (1/2,0,0) x,0,0
(4_{xy}^{-1}|1/2,0,0)

(18) 2 1/4,y,y
(2_{xy}^{-1}|1/2,0,0)

(19) 2 1/4,y,y
(2_{xy}^{-1}|1/2,0,0)

(20) 4^+ (1/2,0,0) x,0,0
(4_{x}|1/2,0,0)

(21) 4^- 1/4,y,-1/4
(4_{xy}^{-1}|1/2,0,0)

(22) 2 (1/4,0,1/4) x+1/4,0,x
(2_{xz}|1/2,0,0)

(23) 4^- 1/4,y,1/4
(4_{xy}^{-1}|1/2,0,0)

(24) 2 (1/4,0,-1/4) x+1/4,0,x
(2_{xz}|1/2,0,0)

(25) 1 0,1/4,1/4
(1|0,1/2,1/2)

(26) b (0,1/2,0) x,y,1/4
(m_{z}|0,1/2,1/2)

(27) c (0,0,1/2) x,1/4,z
(m_{z}|0,1/2,1/2)

(28) n (0,1/2,1/2) 0,y,z
(m_{z}|0,1/2,1/2)

(29) 3^- x,x+1/2;x;
0,1/2,0
(3_{xy}^{-1}|0,1/2,1/2)

(30) 3^- x,x+1/2;x;
0,1/2,0
(3_{xy}^{-1}|0,1/2,1/2)

(31) 3^- x,x+1/2;x;
0,1/2,0
(3_{xy}^{-1}|0,1/2,1/2)

(32) 3^- x,x+1/2;x;
0,1/2,0
(3_{xy}^{-1}|0,1/2,1/2)
For \((1/2,1/2,0) + \text{set}\)

1. \((1/0,0,0)'
   (2) 2' 0,0,0
   (3) 0,0,0'
   (4) 2' x,0,0
   (5) 2' 0,0,0

2. \((1/2,1/2,0) \times x,1/4
   (2) x,1/4,1/4
   (3) 2 (1/2,1/2,0) 1/4,y,0
   (4) 2 (1/2,1/2,0) x,1/4,0

3. \((3/1,3/1,3)
   x+1/6,x+1/3,x
   (3,xyz) 1/2,1/2,0)
   (6) 3' x+1/2,x,x
   (7) 3' x+1/2,x,x
   (8) 3' x+1/2,x,x

4. \((4/1,4/1,4)
   x+1/3,x+1/6,x
   (3,xyz) 1/2,1/2,0)
   (11) 3' (1/3,1/3,-1/3)
   x+1/3,x+1/6,x
   (3,xyz) 1/2,1/2,0)

5. \((2/0,0,0)
   0,0,1/4
   (m,xyz 1/2,1/2,0)
   (3) 0,0,1/4
   (4) 0,0,1/4

6. \((1/2,1/4,0)
   x,1/4,1/4
   (2,xyz 0,1/2,0)
   (11) 3' x,1/4,-1/2,1/4
   (2,xyz 0,1/2,0)

7. \((3/1,4/3)
   x,1/2,1/2,0)
   (3) 0,1/2,1/2,0
   (4) 3' x+1/2,1/2,0

8. \((4/1,0,1/4)
   x+1/4,0,1/4
   (2,xyz 0,1/2,0)
   (23) 4' -1,1/4,y,1/4
   (2,xyz 0,1/2,0)

9. \((2/0,0,0)
   x,1/2,1/2,0)
   (3,xyz 0,1/2,0)
   (27) a (1/2,0,0) x,1/4,0
   (2,xyz 0,1/2,0)

10. \((2/0,0,0)
    x,0,1/2
    (m,xyz 0,1/2,0)
    (3) 0,0,1/4
   (4) 0,0,1/4

11. \((2/0,0,0)
    x,0,1/2
    (m,xyz 0,1/2,0)
    (11) 3' x,1/2,1/2,0
    (2,xyz 0,1/2,0)

12. \((2/0,0,0)
    x,0,1/2
    (m,xyz 0,1/2,0)
    (27) a (1/2,0,0) x,1/4,0
    (2,xyz 0,1/2,0)

13. \((2/0,0,0)
    x,0,1/2
    (m,xyz 0,1/2,0)
    (3) 0,0,1/4
   (4) 0,0,1/4

14. \((2/0,0,0)
    x,0,1/2
    (m,xyz 0,1/2,0)
    (11) 3' x,1/2,1/2,0
    (2,xyz 0,1/2,0)

15. \((2/0,0,0)
    x,0,1/2
    (m,xyz 0,1/2,0)
    (27) a (1/2,0,0) x,1/4,0
    (2,xyz 0,1/2,0)
Continued

(22) $2^\prime (1/2,0,1/2)$ x,1/4,x

(23) $4^\prime (0,1/2,0)$ 0,y,1/2

(24) $2^\prime x+1/2,1/4,x$

(25) $m^\prime x,y,0$

(26) $m^\prime x,0,z$

(27) $m^\prime y,0,0$

(28) $m^\prime 0,y,z$

(29) $3^\prime \cdot x,x,x; 0,0,0$

(30) $3^\prime \cdot x,x; 0,0,0$

(31) $3^\prime \cdot x,x; 0,0,0$

(32) $3^\prime \cdot x,x; 0,0,0$

(33) $3^\prime \cdot x,x,x; 0,0,0$

(34) $3^\prime \cdot x,x,x; 0,0,0$

(35) $3^\prime \cdot x,x,x; 0,0,0$

(36) $3^\prime \cdot x,x,x; 0,0,0$

(37) $0,0,0,0,0$

(38) $n^\prime (1/2,1/2,1/2)$ x,x,z

(39) $4^\prime \cdot 0,1/2,z; 0,1/2,1/4$

(40) $4^\prime \cdot 1/2,0,z; 1/2,0,1/4$

(41) $a^\prime (1/2,0,0)$ x,y+1/2,y

(42) $a^\prime (1/2,0,0)$ x,y+1/2,y

(43) $n^\prime (1/2,1/2,1/2)$ x,y,y

(44) $4^\prime \cdot x,1/2,0,; 1/4,1/2,0$

(45) $b^\prime (0,1/2,0)$ x+1/2,y,x

(46) $b^\prime (0,1/2,0)$ x+1/2,y,x

(47) $4^\prime \cdot 1/2,1/4,0$

(48) $n^\prime (1/2,1/2,1/2)$ x,y,x

(26) $m^\prime 1/4,1/4,0$

(27) $m^\prime 1/2,0,0$

(28) $m^\prime 1/2,0,0$

(29) $3^\prime \cdot x,x+1/2,x; 0,1/2$

(30) $3^\prime \cdot x,x+1/2,x; 0,1/2$

(31) $3^\prime \cdot x,x+1/2,x; 0,1/2$

(32) $3^\prime \cdot x,x+1/2,x; 0,1/2$

(33) $3^\prime \cdot x+1/2,x+1/2,x; 0,0,1/2$

(34) $3^\prime \cdot x+1/2,x+1/2,x; 0,0,1/2$

(35) $3^\prime \cdot x+1/2,x+1/2,x; 0,0,1/2$

(36) $3^\prime \cdot x+1/2,x+1/2,x; 0,0,1/2$

(37) $g^\prime (1/4,-1/4,0)$ x+1/4,x,z

(38) $g^\prime (1/4,1/4,0)$ x+1/4,x,z

(39) $4^\prime \cdot 1/4,1/4,z; 1/4,1/4,0$

(40) $4^\prime \cdot 1/4,1/4,z; 1/4,1/4,0$
Continued

For \( (1/2,0,1/2)' + \) set

\[
\begin{align*}
(1) & \quad t' (1/2,0,1/2) \\
& \quad (1/2,0,1/2)' \\
(2) & \quad 2' (0,0,1/2) \quad 1/4,0,z \\
& \quad (2_2,1/2,0,1/2)' \\
(3) & \quad 2' (1/2,0,0) \quad 1/4,y,1/4 \\
& \quad (2_2,1/2,0,1/2)' \\
(4) & \quad 2' (1/2,0,0) \quad x,0,1/4 \\
& \quad (2_2,1/2,0,1/2)'
\end{align*}
\]

For \( (1/2,1/2,0)' + \) set

\[
\begin{align*}
(1) & \quad t' (1/2,2,1/2) \\
& \quad (1/2,1/2,0)' \\
(2) & \quad 2' (0,0,1/2) \quad 1/4,0,z \\
& \quad (2_2,1/2,2,1/2)' \\
(3) & \quad 2' (1/2,0,0) \quad 1/4,y,1/4 \\
& \quad (2_2,1/2,2,1/2)' \\
(4) & \quad 2' (1/2,0,0) \quad x,0,1/4 \\
& \quad (2_2,1/2,2,1/2)'
\end{align*}
\]
Continued

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<th>Site Symmetry</th>
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<td>(1/2,1/2,0)</td>
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<tr>
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<td>(1/2,0,1/2)</td>
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Generators selected: (1); (1,0,0); (0,1,0); (t(0,0,1)); (t(0,1/2,1/2)); (t(1,2/0,1/2)); (2); (3); (5); (13); (25); 1'.

Positions

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<td>(0,0,0)' +</td>
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<tr>
<td>(0,1/2,1/2,')' +</td>
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<tr>
<td>(1/2,0,1/2)' +</td>
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</tbody>
</table>

226.2.1624 Fm3c1'
Continued

226.2.1624

Fm3c1'

(25) $x, y, z \ [0,0,0]$

(26) $x, y, z \ [0,0,0]$

(27) $x, y, z \ [0,0,0]$

(28) $x, y, z \ [0,0,0]$

(29) $z, x, y \ [0,0,0]$

(30) $z, x, y \ [0,0,0]$

(31) $z, x, y \ [0,0,0]$

(32) $z, x, y \ [0,0,0]$

(33) $y, z, x \ [0,0,0]$

(34) $y, z, x \ [0,0,0]$

(35) $y, z, x \ [0,0,0]$

(36) $y, z, x \ [0,0,0]$

(37) $y + 1/2, x + 1/2, z + 1/2 \ [0,0,0]$

(38) $y + 1/2, x + 1/2, z + 1/2 \ [0,0,0]$

(39) $y + 1/2, x + 1/2, z + 1/2 \ [0,0,0]$

(40) $y + 1/2, x + 1/2, z + 1/2 \ [0,0,0]$

(41) $x + 1/2, z + 1/2, y + 1/2 \ [0,0,0]$

(42) $x + 1/2, z + 1/2, y + 1/2 \ [0,0,0]$

(43) $x + 1/2, z + 1/2, y + 1/2 \ [0,0,0]$

(44) $x + 1/2, z + 1/2, y + 1/2 \ [0,0,0]$

(45) $z + 1/2, y + 1/2, x + 1/2 \ [0,0,0]$

(46) $z + 1/2, y + 1/2, x + 1/2 \ [0,0,0]$

(47) $z + 1/2, y + 1/2, x + 1/2 \ [0,0,0]$

(48) $z + 1/2, y + 1/2, x + 1/2 \ [p$

96  $i \quad m..1'$

$0, y, z \ [0,0,0]$

$0, y, z \ [0,0,0]$

$0, y, z \ [0,0,0]$

$0, y, z \ [0,0,0]$

$z, 0, y \ [0,0,0]$

$z, 0, y \ [0,0,0]$

$z, 0, y \ [0,0,0]$

$z, 0, y \ [0,0,0]$

$y, z, 0 \ [0,0,0]$

$y, z, 0 \ [0,0,0]$

$y, z, 0 \ [0,0,0]$

$y, z, 0 \ [0,0,0]$

$y + 1/2, 1/2, z + 1/2 \ [0,0,0]$

$y + 1/2, 1/2, z + 1/2 \ [0,0,0]$

$y + 1/2, 1/2, z + 1/2 \ [0,0,0]$

$y + 1/2, 1/2, z + 1/2 \ [0,0,0]$

$1/2, z + 1/2, y + 1/2 \ [0,0,0]$

$1/2, z + 1/2, y + 1/2 \ [0,0,0]$

$1/2, z + 1/2, y + 1/2 \ [0,0,0]$

$1/2, z + 1/2, y + 1/2 \ [0,0,0]$

$z + 1/2, y + 1/2, 1/2 \ [0,0,0]$

$z + 1/2, y + 1/2, 1/2 \ [0,0,0]$

$z + 1/2, y + 1/2, 1/2 \ [0,0,0]$

$z + 1/2, y + 1/2, 1/2 \ [0,0,0]$

96  $h  \\quad .21'$

$1/4, y, y \ [0,0,0]$

$3/4, y, y \ [0,0,0]$

$3/4, y, y \ [0,0,0]$

$3/4, y, y \ [0,0,0]$

$y, 1/4, y \ [0,0,0]$

$y, 1/4, y \ [0,0,0]$

$y, 1/4, y \ [0,0,0]$

$y, 1/4, y \ [0,0,0]$

$y, y, 1/4 \ [0,0,0]$

$y, y, 1/4 \ [0,0,0]$

$y, y, 1/4 \ [0,0,0]$

$y, y, 1/4 \ [0,0,0]$

$1/4, y, y \ [0,0,0]$

$1/4, y, y \ [0,0,0]$

$1/4, y, y \ [0,0,0]$

$1/4, y, y \ [0,0,0]$

$3/4, y, y \ [0,0,0]$

$3/4, y, y \ [0,0,0]$

$3/4, y, y \ [0,0,0]$

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$y, y, 3/4 \ [0,0,0]$

$y, y, 3/4 \ [0,0,0]$

64  $g  \quad .3.1'$

$x, x \ [0,0,0]$

$x, x \ [0,0,0]$

$x, x \ [0,0,0]$

$x, x \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$x + 1/2, x + 1/2, x + 1/2 \ [0,0,0]$

$48  f  \\quad .4.1'$

$x, 1/4, 1/4 \ [0,0,0]$

$x, 3/4, 1/4 \ [0,0,0]$

$x, 3/4, 1/4 \ [0,0,0]$

$x, 3/4, 1/4 \ [0,0,0]$

$x, 1/4, 1/4 \ [0,0,0]$

$1/4, x, 1/4 \ [0,0,0]$

$1/4, x, 1/4 \ [0,0,0]$

$1/4, x, 1/4 \ [0,0,0]$

$3/4, x, 1/4 \ [0,0,0]$

$3/4, x, 1/4 \ [0,0,0]$

$3/4, x, 1/4 \ [0,0,0]$

$3/4, x, 1/4 \ [0,0,0]$

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Symmetry of Special Projections

Along [0,0,1] p4mm1'   Along [1,1,1] p6mm1'   Along [1,1,0] p2mm1'
\( a^* = a/2 \quad b^* = b/2 \quad a^* = (2a - b - c)/6 \quad b^* = (-a + 2b - c)/6 \quad a^* = (-a + b)/4 \quad b^* = c/2 \)
Origin at 0,0,z         Origin at x,x,x         Origin at x,x,0
Origin at center (m$^3$)

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/4; \quad y \leq \min(x, 1/2-x); \quad z \leq y\]

Vertices

\[(0,0,0) \quad 1/2,0,0 \quad 1/4,1/4,0 \quad 1/4,1/4,1/4\]

Symmetry Operations

For \((0,0,0) + \) set

\[(1) 1 \quad (1) 0,0,0\]

\[(5) 3^+ x,x,x \quad (6) 3^+ x,x,x \quad (7) 3^+ x,x,x \quad (8) 3^- x,x,x\]

\[(9) 3^- x,x,x \quad (10) 3^- x,x,x \quad (11) 3^- x,x,x \quad (12) 3^- x,x,x\]

\[
\begin{align*}
(5) & \quad (3) x,y,0 \\
& \quad (0,0,0) \\
& \quad (2,0,0) \\
& \quad (3,0,0) \\
& \quad (4,0,0) \\
\end{align*}
\]
(13) $2' (1/2,1/2,0)$ x,$x$,1/4

(14) $2' x,x+1/2,1/4$

(15) $4' (0,0,1/2)$ 1/2,0,2

(16) $4' (0,0,1/2)$ 0,1/2,2

(17) $4' (1/2,0,0)$ x,1/2,0

(18) $2' (0,1/2,0)$ 1/4,$y,y$

(19) $2' 1/4,y+1/2,y$

(20) $4' (1/2,0,0)$ x,0,1/2

(21) $4' (0,1/2,0)$ 1/2,$y,y$

(22) $2' (1/2,1/2,0)$ x,1/4,$x$

(23) $4' (0,1/2,0)$ 0,$y,1/2$

(24) $2' x+1/2,1/4,x$

(25) $1' 0,0,0$

(26) $m' x,y,0$

(27) $m' x,0,z$

(28) $m' 0,y,z$

(29) $3' x,x,x; 0,0,0$

(30) $3' x,x,x; 0,0,0$

(31) $3' x,x,x; 0,0,0$

(32) $3' x,x,x; 0,0,0$

(33) $3' x,x,x; 0,0,0$

(34) $3' x,x,x; 0,0,0$

(35) $3' x,x,x; 0,0,0$

(36) $3' x,x,x; 0,0,0$

(37) $c (0,0,1/2)$ x+1/2,$x,z$

(38) $n (1/2,1/2,1/2)$ x,$x,z$

(39) $4' 0,1/2,z; 0,1/2,1/4$

(40) $4' 1/2,0,z; 1/2,0,1/4$

(41) $4' x,0,1/2; 1/4,0,1/2$

(42) $a (1/2,0,0)$ x,y+1/2,$y$

(43) $n (1/2,1/2,1/2)$ x,y,$y$

(44) $4' x,1/2,0; 1/4,1/2,0$

(45) $4' 0,1/2,0; 0,1/4,1/2$

(46) $b (0,1/2,0)$ x+1/2,$y$,

(47) $4' 1/2,y,0; 1/2,1/4,0$

(48) $n (1/2,1/2,1/2)$ x,$y,x$

For (0,1/2,1/2) + set

(1) $t (0,1/2,1/2)$

(2) $t (0,1/2,1/2)$

(3) $t (0,1/2,1/2)$

(4) $t (0,1/2,1/2)$

(5) $3' (1/3,1/3,1/3)$ x-1/3,x-1/6,$x$

(6) $3' x,x+1/2,$

(7) $3' x+1/3,x-1/6,x$

(8) $3' x+1/2,$

(9) $3' (1/3,1/3,1/3)$ x-1/6,$x+1/6,x$

(10) $3' x+1/2,$

(11) $3' x+1/2,$

(12) $3' x-1/2,$

(13) $2' (1/4,1/4,0)$ x,$x-1/4,0$

(14) $2' x,x+1/4,0$

(15) $4' 1/4,-1/4,z$

(16) $4' 1/4,1/4,z$

(17) $4' (1/2,0,0)$ x,0,0

(18) $2' 1/4,$

(19) $2' y,y$

(20) $4' (1/2,0,0)$ x,0,0

(21) $4' (1/4,0,1/4)$ x,$x+1/4,0$

(22) $2' (1/2,0,0)$

(23) $4' 1/4,1/4$

(24) $2' (1/2,0,0)$

(25) $1' 0,1/2,1/4$

(26) $b' (0,1/2,0)$ x,$y,1/4$

(27) $c (0,0,1/2)$ x,$1/4,z$

(28) $n (0,1/2,1/2)$

(29) $3' x,x+1/2,$

(30) $3' x,x+1/2,$

(31) $3' x,x+1/2,$

(32) $3' x,x+1/2,$

226.3.1625 - 2 - 3772
Continued

226.3.1625

Fm'3c

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
   (1 1/2,1/2,0)

(5) 3' (1/3,1/3,1/3)
   x+1/6,x+1/3,x
   (3xyz |1/2,1/2,0)
   (3xyz |1/2,1/2,0)

(9) 3' (1/3,1/3,1/3)
   x+1/3,x+1/6,x
   (3xyz |1/2,1/2,0)
   (3xyz |1/2,1/2,0)

(13) 2' x,x,1/4
    (2xy |0,0,1/2)
    (2xy |0,0,1/2)

(17) 4' x,1/4,1/4
    (4x |0,0,1/2)
    (4x |0,0,1/2)

(21) 4' 1/4,y,1/4
    (4y |0,0,1/2)
    (4y |0,0,1/2)

(25) 1' 1/4,1/4,0
    (1 1/2,1/2,0)
    (1 1/2,1/2,0)'

(29) 3' x+1/2,x,x;
    (3xyz |1/2,1/2,0)
    (3xyz |1/2,1/2,0)

(33) 3' x,x+1/2;x;
    (3xyz |1/2,1/2,0)
    (3xyz |1/2,1/2,0)

(37) c (0,0,1/2) x,x,z
    (mxy |0,0,1/2)
    (mxy |0,0,1/2)

(41) 4' x,-1/4,1/4; 0,-1/4,1/4
    (4x |0,0,1/2)
    (4x |0,0,1/2)

(45) 4' -1/4,y,1/4; -1/4,0,1/4
    (4y |0,0,1/2)
    (4y |0,0,1/2)

Generators selected
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

192 j 1

(1) x,y,z [u,v,w]
   (2) x,y,z [u,v,w]
   (3) x,y,z [u,v,w]
   (4) x,y,z [u,v,w]

(5) z,x,y [w,u,v]
   (6) z,x,y [w,u,v]
   (7) z,x,y [w,u,v]
   (8) z,x,y [w,u,v]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Case</th>
<th>Projection</th>
<th>2</th>
<th>4'</th>
<th>4'</th>
<th>4'm'</th>
<th>4'm'</th>
<th>m'3'</th>
<th>4'32'</th>
</tr>
</thead>
<tbody>
<tr>
<td>48 f</td>
<td>4'..</td>
<td>x,1/4,1/4 [0,0,0]</td>
<td>x,3/4,1/4 [0,0,0]</td>
<td>1/4,x,1/4 [0,0,0]</td>
<td>1/4,x,3/4 [0,0,0]</td>
<td>1/4,1/4,x [0,0,0]</td>
<td>3/4,1/4,x [0,0,0]</td>
<td>x,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td>48 e</td>
<td>m'm'2..</td>
<td>x,0,0 [u,0,0]</td>
<td>x,0,0 [u,0,0]</td>
<td>0,x,0 [u,0,0]</td>
<td>0,x,0 [u,0,0]</td>
<td>0,0,x [u,0,0]</td>
<td>0,0,x [u,0,0]</td>
<td>1/2,x+1/2,1/2 [u,0,0]</td>
</tr>
<tr>
<td>24 d</td>
<td>4'm'..</td>
<td>0,1/4,1/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
<td>1/4,0,1/4 [0,0,0]</td>
<td>1/4,0,3/4 [0,0,0]</td>
<td>1/4,0,3/4 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
</tr>
<tr>
<td>24 c</td>
<td>4'm'2'</td>
<td>1/4,0,0 [u,0,0]</td>
<td>3/4,0,0 [u,0,0]</td>
<td>3/4,0,0 [u,0,0]</td>
<td>0,1/4,0 [u,0,0]</td>
<td>0,3/4,0 [u,0,0]</td>
<td>0,3/4,0 [u,0,0]</td>
<td>0,0,1/4 [0,0,u]</td>
</tr>
<tr>
<td>8 b</td>
<td>m'3'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td>8 a</td>
<td>4'32'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

- **Along [0,0,1]**: \( p4'm'm \)
  - \( a^* = a/2 \)
  - \( b^* = b/2 \)
  - Origin at 0,0,z

- **Along [1,1,1]**: \( p6mm \)
  - \( a^* = (2a - b - c)/6 \)
  - \( b^* = (-a + 2b - c)/6 \)
  - Origin at x,x,x

- **Along [1,1,0]**: \( p2mm1' \)
  - \( a^* = (-a + b)/4 \)
  - \( b^* = c/2 \)
  - Origin at x,x,0
**Origin** at center (m\(3\))

**Asymmetric unit**

- \(0 \leq x \leq 1/2;\)
- \(0 \leq y \leq 1/4;\)
- \(0 \leq z \leq 1/4;\)
- \(y \leq \min(x, 1/2-x);\)
- \(z \leq y\)

**Vertices**

- \(0,0,0\)
- \(1/2,0,0\)
- \(1/4,1/4,0\)
- \(1/4,1/4,1/4\)

**Symmetry Operations**

For \((0,0,0) + \text{set}\)

1. \((1) 1\)
2. \((2) 2 \ 0,0,z\)
3. \((3) 2 \ 0,y,0\)
4. \((4) 2 \ x,0,0\)
5. \((5) 3^+ \ x,x,x\)
   \(\left(3_{xyz}\right)0,0,0\)
6. \((6) 3^+ \ x,x,x\)
   \(\left(3_{xyz}^{-1}\right)0,0,0\)
7. \((7) 3^+ \ x,x,x\)
   \(\left(3_{xyz}^{-1}\right)0,0,0\)
8. \((8) 3^+ \ x,x,x\)
   \(\left(3_{xyz}^{-1}\right)0,0,0\)
9. \((9) 3^- \ x,x,x\)
   \(\left(3_{xyz}\right)0,0,0\)
10. \((10) 3^- \ x,x,x\)
    \(\left(3_{xyz}\right)0,0,0\)
11. \((11) 3^- \ x,x,x\)
    \(\left(3_{xyz}\right)0,0,0\)
12. \((12) 3^- \ x,x,x\)
    \(\left(3_{xyz}\right)0,0,0\)
(33) $\bar{3}' x-1/2, x-1/2, x$; $0,0,1/2$ 
(3) $\bar{3}' x+1/2, x-1/2, x$; $0,0,1/2$ 
(3) $\bar{3}' x-1/2, x+1/2, x$; $-1/2,1/2,0$ 
(3) $\bar{3}' x+1/2, x+1/2, x$; $1/2,1/2,0$

(37) $g'(1/4,-1/4,0) x+1/4, x, z$  
(38) $g'(1/4,1/4,0) x+1/4, x, z$  
(39) $4^{*} -1/4,1/4, z; 1/4,1/4,0$  
(40) $4^{*} -1/4,1/4, z; 1/4,1/4,0$

(41) $\bar{4}' -1,0,0; 1/4,0,0$  
(42) $a'(1/2,0,0) y, y, y$  
(43) $a'(1/2,0,0) y, y, y$  
(44) $4^{*} x, 0,0; 1/4,0,0$

(45) $4^{*} -1,4,1/4; 1/4,0,1/4$  
(46) $g'(1/4,0,-1/4) x+1, y, x$  
(47) $4^{*} -1,4, y,-1/4; 1/4,0,-1/4$  
(48) $g'(1/4,0,1/4) x+1, y, x$

For $(1/2,0,1/2) + \text{set}$

(1) $t (1/2,0,1/2) + \text{set}$
(2) $2 (0,0,1/2) 1/4,0, z$  
(3) $2 y 1/4,1/4, z$  
(4) $2 (1,2,0,1/2) 0,1/4,0$

(5) $3^{1} (3,1,3,1/3)$ $x+1/6, x+1/6, x$  
(6) $3^{1} (3,1,3,1/3)$ $x+1/6, x+1/6, x$  
(7) $3^{1} x+1/2, x+1/2, x$  
(8) $3^{1} x+1/2, x+1/2, x$  

(9) $3 (1,3,1,3)$ $x+1/6, x+1/3, x$  
(10) $3^{1} x+1/2, x+1/2, x$  
(11) $3^{1} x+1/2, x+1/2, x$  
(12) $3 (1,3,1,3)$ $x+1/6, x+1/3, x$

(13) $2^{1} (1/4,1/4,0) x, x+1/4,0$  
(14) $2^{1} (1/4,1/4,0) x, x+1/4,0$  
(15) $4^{*} -1/4,1/4, z$  
(16) $4^{*} -1,4,1/4, z$

(17) $4^{*} x, 1/4,-1/4$  
(18) $2^{1} (0,1/4,1/4) 0, y+1, y$  
(19) $2^{1} (0,1/4,1/4) 0, y+1, y$  
(20) $4^{*} x, 1,4,1/4$

(21) $4^{*} (0,1/2,0) 0, y, 0$  
(22) $2^{1} x, 1/4, x$  
(23) $4^{*} (0,1/2,0) 0, y, 0$  
(24) $2^{1} x, 1/4, x$

(25) $t (1/4,0,1/4) 1/4,0,1/4$  
(26) $a (1/2,0,0) x, y, 1/4$  
(27) $n (1/2,0,1/2) 0, x, 0$  
(28) $c (0,0,1/2) 1/4, y, z$

(29) $3^{1} x-1/2, x-1/2, x$  
(30) $3^{1} x-1/2, x-1/2, x$  
(31) $3^{1} x+1/2, x+1/2, x$  
(32) $3^{1} x+1/2, x+1/2, x$

(33) $3^{1} x+1/2, x, x$  
(34) $3^{1} x+1/2, x, x$  
(35) $3^{1} x+1/2, x, x$  
(36) $3^{1} x+1/2, x, x$

(37) $g'(-1/4,1/4,0) x+1/4, x, z$  
(38) $g'(1/4,1/4,0) x+1/4, x, z$  
(39) $4^{*} -1/4,1/4, z; -1/4,1/4,0$  
(40) $4^{*} -1/4,1/4, z; -1/4,1/4,0$

(41) $4^{*} x, 1/4,1/4; 0,1/4,1/4$  
(42) $g'(0,1/4,1/4) x, y+1/4, y$  
(43) $g'(0,1/4,1/4) x, y+1/4, y$  
(44) $4^{*} x, 1/4,-1/4; 0,1/4,-1/4$

(45) $4^{*} y, 0, 0; 0,1/4,0$  
(46) $b' (0,1/2,0) x, y, x$  
(47) $4^{*} y, 0, 0; 0,1/4,0$  
(48) $b' (0,1/2,0) x, y, x$
Continued 226.4.1626 Fm\(3c'\) & 226.4.1626 & Fm\(3c'\) \\
For \((1/2,1/2,0) + \) set \\
\begin{align*}
(1) & t \ (1/2,1/2,0) \\
(2) & 2 \ 1/4,1/4,z \\
(3) & 2 \ (0,1/2,0) \ 1/4,y,0 \\
(4) & 2 \ (1/2,0,0) \ x,1/4,0 \\
(5) & 3^* \ (1/3,1/3,1/3) \\
(6) & 3^* \ x+1/2,x,x \\
(7) & 3^* \ x+1/2,x,x \\
(8) & 3^* \ (1/3,1/3,-1/3) \\
(9) & 3 \ (1/3,1/3,1/3) \\
(10) & 3 \ x,x+1/2,x \\
(11) & 3 \ (1/3,1/3,-1/3) \\
(12) & 3 \ x,x+1/2,x \\
(13) & 2' \ x,x,1/4 \\
(14) & 2' \ x,x,1/4 \\
(15) & 4' \ (0,0,1/2) \ 0,0,z \\
(16) & 4' \ (0,0,1/2) \ 0,0,z \\
(17) & 4' \ x,1/4,1/4 \\
(18) & 2' \ (0,1/4,1/4) \ 0,y-1/4,y \\
(19) & 2' \ (0,-1/4,1/4) \ 0,y+1/4,y \\
(20) & 4' \ (-1/4,1/4,1/4) \\
(21) & 4' \ -1/4,y,1/4 \\
(22) & 2' \ (-1/4,0,1/4) \ x-1/4,y,x \\
(23) & 4' \ -1/4,y,1/4 \\
(24) & 2' \ (-1/4,0,1/4) \ x+1/4,0,x \\
(25) & 1/4,1/4,0 \\
(26) & n \ (1/2,1/2,0) \\
(27) & a \ (1/2,0,0) \ x,1/4,z \\
(28) & b \ (0,1/2,0) \ 1/4,y,z \\
(29) & 3^* \ x+1/2,x,x; \\
(30) & 3^* \ x-1/2,x,x; \\
(31) & 3^* \ x-1/2,x,x; \\
(32) & 3^* \ x+1/2,x,x; \\
(33) & 3^* \ x+1/2,x,x; \\
(34) & 3^* \ x+1/2,x,x; \\
(35) & 3^* \ x+1/2,x,x; \\
(36) & 3^* \ x+1/2,x,x; \\
(37) & c' \ (0,0,1/2) \ x,x,z \\
(38) & c' \ (0,0,1/2) \ x,x,z \\
(39) & 4' \ (0,0,1/2) \ 0,0,z; \\
(40) & 4' \ (0,0,1/2) \ 0,0,z; \\
(41) & 4' \ x-1/4,1/4; \\
(42) & g' \ (0,-1/4,1/4) \ x,y+1/4,y \\
(43) & g' \ (0,1/4,1/4) \ x,y-1/4,y \\
(44) & 4' \ x,1/4,1/4; \\
(45) & 4' \ -1/4,y,1/4; \\
(46) & g' \ (1/4,0,1/4) \ x+1/4,y,x \\
(47) & 4' \ 1/4,y,1/4; \\
(48) & g' \ (1/4,0,1/4) \ x-1/4,y,x \\
\end{align*}

Generators selected \((1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,0); (2); (3); (5); (13); (25).\)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>192 j 1</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
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</tbody>
</table>

\((1) \ x,y,z \ [u,v,w] \ (2) \ x,y,z \ [u,v,w] \ (3) \ x,y,z \ [u,v,w] \ (4) \ x,y,z \ [u,v,w] \ (5) \ z,x,y \ [w,u,v] \ (6) \ z,x,y \ [w,u,v] \ (7) \ z,x,y \ [w,u,v] \ (8) \ z,x,y \ [w,u,v] \)
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>48 f</th>
<th>4'..</th>
<th>x,1/4,1/4 [0,0,0]</th>
<th>x,3/4,1/4 [0,0,0]</th>
<th>1/4,x,1/4 [0,0,0]</th>
<th>1/4,x,3/4 [0,0,0]</th>
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<tbody>
<tr>
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<td></td>
<td>1/4,1/4,x [0,0,0]</td>
<td>3/4,1/4,x [0,0,0]</td>
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<td>3/4,x,3/4 [0,0,0]</td>
<td>3/4,x,1/4 [0,0,0]</td>
<td>3/4,3/4,x [0,0,0]</td>
<td>1/4,3/4,x [0,0,0]</td>
</tr>
<tr>
<td>48 e</td>
<td>mm2..</td>
<td>x,0,0 [0,0,0]</td>
<td>x,0,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
<td>0,x,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,0,x [0,0,0]</td>
<td>0,0,x [0,0,0]</td>
<td>1/2,x+1/2,1/2 [0,0,0]</td>
<td>1/2,x+1/2,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x+1/2,1/2,1/2 [0,0,0]</td>
<td>x+1/2,1/2,1/2 [0,0,0]</td>
<td>1/2,1/2,x+1/2 [0,0,0]</td>
<td>1/2,1/2,x+1/2 [0,0,0]</td>
</tr>
<tr>
<td>24 d</td>
<td>4'/m..</td>
<td>0,1/4,1/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
<td>1/4,0,1/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1/4,0,3/4 [0,0,0]</td>
<td>1/4,1/4,0 [0,0,0]</td>
<td>3/4,1/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>24 c</td>
<td>4'm.2'</td>
<td>1/4,0,0 [0,0,0]</td>
<td>3/4,0,0 [0,0,0]</td>
<td>0,1/4,0 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0,3/4,0 [0,0,0]</td>
<td>0,0,1/4 [0,0,0]</td>
<td>0,0,3/4 [0,0,0]</td>
<td></td>
</tr>
<tr>
<td>8 b</td>
<td>m3.</td>
<td>0,0,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 a</td>
<td>4'32'</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0,0,1]**: p4mm1'  
  \( a^* = a/2 \)  \( b^* = b/2 \)  
  Origin at 0,0,z

- **Along [1,1,1]**: p6'mm'  
  \( a^* = (2a - b - c)/6 \)  \( b^* = (-a + 2b - c)/6 \)  
  Origin at x,x,x

- **Along [1,1,0]**: p2mm'  
  \( a^* = c/2 \)  \( b^* = -(a + b)/4 \)  
  Origin at x,x,0

---

226.4.1626 - 6 - 3782
Origin at center (m'3')

Asymmetric unit
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/4; \quad 0 \leq z \leq 1/4; \quad y \leq \min(x,1/2-x); \quad z \leq y\]

Vertices
\[0,0,0 \quad 1/2,0,0 \quad 1/4,1/4,0 \quad 1/4,1/4,1/4\]

Symmetry Operations

For \((0,0,0) + \) set

\[(1) \begin{array}{c} 1 \\ (1) 0,0,0 \end{array} \]

\[(2) \begin{array}{c} 2 \quad 0,0,z \\ (2) 0,0,0 \end{array} \]

\[(3) \begin{array}{c} 2 \quad 0,y,0 \\ (2) 0,0,0 \end{array} \]

\[(4) \begin{array}{c} 2 \quad x,0,0 \\ (2) 0,0,0 \end{array} \]

\[(5) \begin{array}{c} 3^+ \quad x,x,x \\ (3_{xyz}0,0,0) \end{array} \]

\[(6) \begin{array}{c} 3^+ \quad x,x,x \\ (3_{xyz}0,0,0) \end{array} \]

\[(7) \begin{array}{c} 3^+ \quad x,x,x \\ (3_{xyz}0,0,0) \end{array} \]

\[(8) \begin{array}{c} 3^+ \quad x,x,x \\ (3_{xyz}0,0,0) \end{array} \]

\[(9) \begin{array}{c} 3^- \quad x,x,x \\ (3_{xyz}^{-1}0,0,0) \end{array} \]

\[(10) \begin{array}{c} 3^- \quad x,x,x \\ (3_{xyz}^{-1}0,0,0) \end{array} \]

\[(11) \begin{array}{c} 3^- \quad x,x,x \\ (3_{xyz}0,0,0) \end{array} \]

\[(12) \begin{array}{c} 3^- \quad x,x,x \\ (3_{xyz}0,0,0) \end{array} \]
| (13) | $2 \begin{pmatrix} 1/2,1/2,0 \end{pmatrix}$ | $0,0,0$ | $0,1/2,1/2$ |
| (14) | $2 \begin{pmatrix} x, x+1/2,1/4 \end{pmatrix}$ | $0,0,0$ | $0,1/2,1/2$ |
| (15) | $4 \begin{pmatrix} 0,0,1/2 \end{pmatrix}$ | $1/2,0,z$ | $1/2,0,z$ |
| (16) | $4 \begin{pmatrix} 0,1/2,0 \end{pmatrix}$ | $1/2,0,z$ | $1/2,0,z$ |
| (17) | $4 \begin{pmatrix} 1/2,0,0 \end{pmatrix}$ | $x,1/2,0$ | $1/2,1/2,1/2$ |
| (18) | $2 \begin{pmatrix} 0,1/2,1/2 \end{pmatrix}$ | $1/4, y, y$ | $1/2,1/2,1/2$ |
| (19) | $2 \begin{pmatrix} 1/4, y+1/2, y \end{pmatrix}$ | $1/2,1/2,1/2$ | $1/2,1/2,1/2$ |
| (20) | $4 \begin{pmatrix} 1/2,0,0 \end{pmatrix}$ | $x,0,1/2$ | $1/2,1/2,1/2$ |
| (21) | $4 \begin{pmatrix} 0,1/2,0 \end{pmatrix}$ | $0,1/2,0$ | $1/2,1/2,1/2$ |
| (22) | $2 \begin{pmatrix} 1/2,0,1/2 \end{pmatrix}$ | $x,1/4, x$ | $1/2,1/2,1/2$ |
| (23) | $4 \begin{pmatrix} 0,1/2,0 \end{pmatrix}$ | $0,1/2,1/2$ | $1/2,1/2,1/2$ |
| (24) | $2 \begin{pmatrix} x, x+1/2,1/4 \end{pmatrix}$ | $1/2,1/2,1/2$ | $1/2,1/2,1/2$ |

Continued
Continued

(33) $\overline{3}'$ x-1/2, x-1/2, x;
$\overline{3}'$ x+1/2, x-1/2, x;
$\overline{3}'$ x-1/2, x+1/2, x;

$\overline{3}'$ x+1/2, x+1/2, x;

(34) $\overline{3}'$ x+1/2, x-1/2, x;
$\overline{3}'$ x-1/2, x+1/2, x;

$\overline{3}'$ x+1/2, x+1/2, x;

(35) $\overline{3}'$ x-1/2, x+1/2, x;
$\overline{3}'$ x-1/2, x+1/2, x;

$\overline{3}'$ x+1/2, x+1/2, x;

(36) $\overline{3}'$ x+1/2, x+1/2, x;

$\overline{3}'$ x+1/2, x+1/2, x;

(37) $g'$ (1/4, -1/4, 0) x+1/4, x, z

(38) $g'$ (1/4, 1/4, 0) x+1/4, x, z

(39) $4'$ 1/4, 1/4, z; 1/4, 1/4, 0

$4'$ 1/4, 1/4, z; 1/4, 1/4, 0

(40) $4'$ 1/4, -1/4, z; 1/4, -1/4, 0

$4'$ 1/4, -1/4, z; 1/4, -1/4, 0

(41) $4'$ x, 0, 0; 1/4, 0, 0

$4'$ x, 1/4, -1/4

$4'$ x, 1/4, -1/4

(42) $g'$ (1/2, 0, 0) x, y, y

$4'$ x, 1/4, -1/4

$4'$ x, 1/4, -1/4

(43) $a'$ (1/2, 0, 0) x, y, y

$4'$ x, 1/4, -1/4

$4'$ x, 1/4, -1/4

(44) $4'$ x, 0, 0; 1/4, 0, 0

$4'$ x, 0, 0; 1/4, 0, 0

(45) $4'$ 1/4, y, 1/4; 1/4, 0, 1/4

$4'$ 1/4, y, 1/4; 1/4, 0, 1/4

$4'$ 1/4, y, 1/4; 1/4, 0, 1/4

(46) $g'$ (1/4, 0, -1/4) x+1/4, y, x

$4'$ 1/4, y, 1/4; 1/4, 0, 1/4

$4'$ 1/4, y, 1/4; 1/4, 0, 1/4

(47) $4'$ 1/4, y, -1/4; 1/4, 0, -1/4

$4'$ 1/4, y, -1/4; 1/4, 0, -1/4

$4'$ 1/4, y, -1/4; 1/4, 0, -1/4

(48) $g'$ (1/4, 0, 1/4) x+1/4, y, x

$4'$ 1/4, y, -1/4; 1/4, 0, -1/4

$4'$ 1/4, y, -1/4; 1/4, 0, -1/4

For (1/2, 0, 1/2) + set

(1) $t$ (1/2, 0, 1/2)

(2) 2 (0, 0, 1/2)

(3) 2 (1/4, y, 1/4)

(4) 2 (1/2, 0, 0)

(1/2, 0, 1/2)

(2) 2 (1/2, 0, 1/2)

(3) 2 (1/2, 0, 1/2)

(4) 2 (1/2, 0, 1/2)

(5) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

(6) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

(7) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

(8) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

(9) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

(10) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

(11) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

(12) $3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)

$3'$ (1/3, 1/3, 1/3)
Continued

226.5.1627  Fm’3c’

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(1/2,1/2,0)
(2) 2 1/4,1/4,z
(2) |1/2,1/2,0)
(3) 2 (0,1/2,0) 1/4,y,0
(3) |1/2,1/2,0)
(4) 2 (1/2,0,0) x,1/4,0
(4) |1/2,1/2,0)
(5) 3* (1/3,1/3,1/3) x+1/6,x+1/3,x
(3) |1/2,1/2,0)
(6) 3* x+1/2,x,x
(3) |1/2,1/2,0)
(7) 3* x+1/2,x,x
(3) |1/2,1/2,0)
(8) 3* (1/3,1/3,-1/3) x+1/6,x+1/3,x
(3) |1/2,1/2,0)
(9) 3* (1/3,1/3,1/3) x+1/3,x+1/6,x
(3) |1/2,1/2,0)
(10) 3* x,x+1/2,x
(3) |1/2,1/2,0)
(11) 3* (1/3,1/3,-1/3) x+1/3,x+1/6,x
(3) |1/2,1/2,0)
(12) 3* x,x+1/2,x
(3) |1/2,1/2,0)
(13) 2 x,x,1/4
(2) |0,0,1/2)
(14) 2 x,x,1/4
(2) |0,0,1/2)
(15) 4* (0,0,1/2) 0,0,z
(4) |0,0,1/2)
(16) 4* (0,0,1/2) 0,0,z
(4) |0,0,1/2)
(17) 4* x,1/4,1/4
(2) |0,0,1/2)
(18) 2 (0,1/4,1/4) 0,y-1/4,y
(2) |0,0,1/2)
(19) 2 (0,-1/4,1/4) 0,y+1/4,y
(2) |0,0,1/2)
(20) 4* x,-1/4,1/4
(2) |0,0,1/2)
(21) 4* 1/4,1/4,1/4
(2) |0,0,1/2)
(22) 2 (1/4,0,1/4) x-1/4,0,x
(2) |0,0,1/2)
(23) 4* -1/4,1/4,1/4
(2) |0,0,1/2)
(24) 2 (-1/4,0,1/4) x+1/4,0,x
(2) |0,0,1/2)
(25) 1' 1/4,1/4,0
(1) |1/2,1/2,0)
(26) n' (1/2,1/2,0) x,y,0
(26) |1/2,1/2,0)
(27) a' (1/2,0,0) x,1/4,z
(27) |1/2,1/2,0)
(28) b' (0,1/2,0) 1/4,y,z
(28) |1/2,1/2,0)
(29) 3' x+1/2,x,x;
(3) |1/2,1/2,0)
(30) 3' x+1/2,x+1/2,x;
(3) |1/2,1/2,0)
(31) 3' x+1/2,x+1/2,x;
(3) |1/2,1/2,0)
(32) 3' x+1/2,x+1/2,x;
(3) |1/2,1/2,0)
(33) 3' x+1/2,x+1/2,x+1/2;
(3) |1/2,1/2,0)
(34) 3' x+1/2,x+1/2,x;
(3) |1/2,1/2,0)
(35) 3' x+1/2,x+1/2,x;
(3) |1/2,1/2,0)
(36) 3' x+1/2,x+1/2,x;
(3) |1/2,1/2,0)
(37) c' (0,0,1/2) x,x,z
(3) |0,0,1/2)
(38) c' (0,0,1/2) x,x,z
(3) |0,0,1/2)
(39) 4* 1/4,0,1/4
(4) |0,0,1/2)
(40) 4* 1/4,0,1/4
(4) |0,0,1/2)
(41) 4* 1/4,0,1/4
(4) |0,0,1/2)
(42) 4* 1/4,0,1/4
(4) |0,0,1/2)
(43) 4* 1/4,0,1/4
(4) |0,0,1/2)
(44) 4* 1/4,0,1/4
(4) |0,0,1/2)
(45) 4* 1/4,0,1/4
(4) |0,0,1/2)
(46) 4* 1/4,0,1/4
(4) |0,0,1/2)
(47) 4* 1/4,0,1/4
(4) |0,0,1/2)
(48) 4* 1/4,0,1/4
(4) |0,0,1/2)

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions Coordinates

Multiplicity, Wyckoff letter, Site Symmetry.

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(1) x,y,z [u,v,w]
(2) x,y,z [u,v,w]
(3) x,y,z [u,v,w]
(4) x,y,z [u,v,w]
(5) z,x,y [w,u,v]
(6) z,x,y [w,u,v]
(7) z,x,y [w,u,v]
(8) z,x,y [w,u,v]
Continued

48  f  4..  x,1/4,1/4 [u,0,0]  \( \tilde{x},3/4,1/4 [u,0,0] \)  \( 1/4,x,1/4 [0,u,0] \)  \( 1/4,\tilde{x},3/4 [0,\tilde{u},0] \)  
   1/4,1/4,x [u,0,u]  3/4,1/4,\tilde{x} [0,0,\tilde{u}]  \( \tilde{x},3/4,3/4 [u,0,0] \)  \( x,1/4,3/4 [u,0,0] \)  
   3/4,\tilde{x},3/4 [0,\tilde{u},0]  3/4,\tilde{x},1/4 [0,u,0]  \( 3/4,3/4,\tilde{x} [0,0,\tilde{u}] \)  \( 1/4,3/4,x [0,u,0] \)  

48  e  m'm'2..  x,0,0 [u,0,0]  \( \tilde{x},0,0 [u,0,0] \)  0,0,x [u,0,0]  \( 0,\tilde{x},0 [0,\tilde{u},0] \)  
   x+1/2,1/2,1/2 [u,0,u]  \( \tilde{x}+1/2,1/2,1/2 [u,0,u] \)  \( 1/2,\tilde{x}+1/2,1/2 [0,\tilde{u},0] \)  \( 1/2,\tilde{x}+1/2,1/2 [0,\tilde{u},0] \)  

24  d  4/m'.  0,1/4,1/4 [0,0,0]  0,3/4,1/4 [0,0,0]  \( 1/4,0,1/4 [0,0,0] \)  
   1/4,0,3/4 [0,0,0]  1/4,1/4,0 [0,0,0]  \( 3/4,1/4,0 [0,0,0] \)  

24  c  \( \overline{4} \)m'.2  1/4,0,0 [0,0,0]  3/4,0,0 [0,0,0]  \( 0,1/4,0 [0,0,0] \)  
   0,3/4,0 [0,0,0]  \( 0,0,1/4 [0,0,0] \)  \( 0,0,3/4 [0,0,0] \)  

8  b  m'\( \overline{3} \).  0,0,0 [0,0,0]  \( 1/2,1/2,1/2 [0,0,0] \)  

8  a  432  1/4,1/4,1/4 [0,0,0]  \( 3/4,3/4,3/4 [0,0,0] \)  

**Symmetry of Special Projections**

Along [0,0,1] p4m'm'
\( a^* = a/2 \)  \( b^* = b/2 \)  
Origin at 0,0,z

Along [1,1,1] p6m'm'
\( a^* = (2a - b - c)/6 \)  \( b^* = (-a + 2b - c)/6 \)  
Origin at x,x,x

Along [1,1,0] p2m'm'
\( a^* = (-a + b)/4 \)  \( b^* = c/2 \)  
Origin at x,x,0
Origin at $\overline{4}3m$, at -1/8,-1/8,-1/8 from center ($\overline{3}m$)

Asymmetric unit:
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/8; \quad -1/8 \leq z \leq 1/8; \quad y \leq \min(1/2-x, x); \quad -y \leq z \leq y\]

Vertices:
0,0,0 \quad 1/2,0,0 \quad 3/8,1/8,1/8 \quad 1/8,1/8,1/8 \quad 3/8,1/8,-1/8 \quad 1/8,1/8,-1/8

Symmetry Operations

For (0,0,0) + set

(1) 1
(2) 2 (0,0,1/2) 0,1/4,z
   $\overline{2}z$ 0,1/2,1/2

(5) $3^+$ x,x,x
   $3^+$ (1/3,-1/3,1/3)
   $x+1/6,x+1/6,x$
   $3_{xyz}^{-1}$ 1/2,0,1/2

(9) $3^-$ x,x,x
   $3^-$ (0,0,0)
   $3^-$ (1/3,1/3,-1/3)
   $x+1/6,x+1/3,x$
   $3_{xyz}^{-1}$ 1/2,1/2,0

(3) 2 (0,1/2,0) 1/4,y,0
   $\overline{2}y$ 1/2,1/2,0

(6) $3^+$ x,x,x
   $3^+$ (1/3,-1/3,1/3)
   $x+1/3,x-1/6,x$
   $3_{xyz}^{-1}$ 0,1/2,1/2

(7) $3^-$ x,x,x
   $3^-$ (1/3,1/3,-1/3)
   $x+1/6,x+1/3,x$
   $3_{xyz}^{-1}$ 1/2,1/2,0

(10) $3^-$ x,x,x
   $3^-$ (1/3,1/3,-1/3)
   $x+1/6,x+1/3,x$
   $3_{xyz}^{-1}$ 1/2,1/2,0

(11) $3^-$ x,x,x
   $3^-$ (1/3,1/3,-1/3)
   $x+1/6,x+1/3,x$
   $3_{xyz}^{-1}$ 1/2,1/2,0

(12) $3^-$ x,x,x
   $3^-$ (1/3,1/3,-1/3)
   $x+1/6,x+1/3,x$
   $3_{xyz}^{-1}$ 1/2,1/2,0

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(13) 2 (1/2,1/2,0) x,x-1/4,3/8
(2,xy \ |3/4,1/4,3/4)

(17) 4e (3/4,0,0) x,1/2,1/4
(4,xy \ |3/4,1/4,3/4)

(21) 4e (0,1/4,0) 3/4,y,0
(4,xy \ |3/4,1/4,3/4)

(25) \( \overline{1} 1/8,1/8,1/8
(1 |1/4,1/4,1/4)

(29) 3e x,x,x;
(3,xyz |1/4,1/4,1/4)

(33) 3e x,x,x;
(3,xyz |1/4,1/4,1/4)

(37) g (1/4,-1,1/4,1/2) x+1/4,x,z
(m,xyz |0,2,0,1/2)

(41) 4e x,-1/4,1/4; 1/4,-1,1/4,1/4
(4e |1/2,0,1/2)

For (0,1/2,1/2) + set

(1) t (0,1/2,1/2)
(1 |0,1/2,1/2)

(5) 3e (1/3,1/3,1/3)

x-1/3,x-1/6,x
(3,xyz |0,1/2,1/2)

(9) 3e (1/3,1/3,1/3)

x-1/6,x+1/6,x
(3,xyz |0,1/2,1/2)

(13) 2 (3/4,3/4,0) x,x,1/8
(2,xy |3/4,3/4,1/4)

(17) 4e (3/4,0,0) x,1/2,-1/4
(4,xy |3/4,3/4,1/4)

(21) 4e (0,3/4,0) 1/2,y,-1/4
(4,xy |3/4,3/4,1/4)

(25) \( \overline{1} 1/8,3/8,3/8
(1 |1/4,3/4,3/4)

(29) 3e x,x+1/2,x;
(3,xyz |1/4,3/4,3/4)

227.1.1628 - Fd3m
For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
   (1) 1/2,1/2,0)
(2) 2 (0,0,1/2) 1/4,0,z
   (2) 1/2,0,1/2)
(3) 2 0,y,0
(4) 2 x,1/4,1/4
   (2,0,1/2,1/2)
(5) 3*(1/3,1/3,1/3)
   x+1/6,x+1/3,x
   (3,1/2,1/2,0)
(6) 3* x,x+1/2,x
   (3,xyz 1,0,1/2)
(7) 3* x+1/2,x-1/2,x
   (3,xyz 1,0,1/2)
(8) 3* x,x,x
(9) 3* (1/3,1/3,1/3)
   x+1/3,x+1/6,x
   (3,xyz -1 1/2,1/2,0)
(10) 3* x,x,x
   (3,xyz 0,0,0)
(11) 3* x+1/2,x+1/2,x
   (3,xyz 0,1/2,1/2)
(12) 3* (1/3,1/3,1/3)
   x-1/6,x+1/3,x
   (3,xyz 1,0,1/2)
(13) 2 (1/2,1/2,0) x,x+1/4,3/8
   (2,xyz 1/4,3/4,1/4)
(14) 2 x,x+3/4,1/8
   (2,xyz 3/4,3/4,1/4)
(15) 4* (0,0,3/4) 1/2,-1/4,z
   (4,xyz 3/4,1,4/4)
(16) 4* (0,0,1/4) 0,1/4,z
   (4,xyz 1/4,1,4/4)
(17) 4* (1/4,0,0) x,3/4,0
   (4,xyz -1 1/4,3,4/4)
(18) 2 (0,1/4,1/4) 1/8,y,y
   (2,xyz 1,0,1/2)
(19) 2 (0,1/4,-1/4) 3/8,y+1/2,y
   (2,xyz 3/4,3,4/4)
(20) 4* (3,4,0,0) x,-1/4,1/2
   (4,xyz 1/4,1,4/4)
(21) 4* (0,3/4,0) 1/2,y,1/4
   (4,xyz 1,0,1/2)
(22) 2 (3/4,0,3/4) x,1/8,x
   (2,xyz 3/4,1,4/4)
(23) 4* (0,1/4,0) 0,y,1/4
   (4,xyz 1,1/4,4/4)
(24) 2 (1/4,-3/4) x+1/2,3/8,x
   (2,xyz 3/4,3,4/4)
(25) 3+ 1/2,1/2,1/2
   (1/2,1/2,1/2)
(26) 6 d (3/4,1/4,0) x,y,3/8
   (m,xyz 1/4,3,4/4)
(27) d (1/4,0,1/4) x,1/8,z
   (m,xyz 1/4,1,4/4)
(28) d (0,3/4,3/4) 1/8,y,z
   (m,xyz 1/4,3,4/4)
(29) 3* x+1/2,x,x;
   5/8,1/8,1/8
   (3,xyz 1/4,3,4/4)
(30) 3* x-3/2,x+1,x;
   -5/8,1/8,7/8
   (3,xyz -1 1/4,3,4/4)
(31) 3* x+1/2,x+1,x;
   5/8,7/8,1/8
   (3,xyz -1 1/4,3,4/4)
(32) 3* x+1/2,x,x;
   3/8,1/8,1/8
   (3,xyz -1 1/4,3,4/4)
(33) 3* x,x+1/2,x;
   1/8,5/8,1/8
   (3,xyz -1 1/4,3,4/4)
(34) 3* x+1/2,x-1/2,x;
   1/8,-1/8,3/8
   (3,xyz 1/4,1,4/4)
(35) 3* x-1/2,x+1,x;
   -5/8,7/8,1/8
   (3,xyz 1/4,3,4/4)
(36) 3* x+1,x,x;
   7/8,1/8,-1/8
   (3,xyz 1/4,3,4/4)
(37) g (-1/4,1/4,1/2) x+1/4,x,z
   (m,xyz 0,1/2,1/2)
(38) g (1/2,1/2,0) x,x,z
   (m,xyz 1/2,1/2,0)
(39) 4* 1/4,1/4,z; 1/4,1/4,1/4
   (4,xyz 1/2,0,1/2)
(40) 4* 0,0,z; 0,0,0
   (4,xyz 0,0,0)
(41) 4* x,0,1/2; 0,0,1/2
   (4,xyz 0,1/2,1/2)
(42) m x,y,y
   (m,xyz 0,0,0)
(43) g (1/2,1/4,1/4) x,y+1/4,y
   (m,xyz 1/2,1/2,0)
(44) 4* x,1/4,1/4; 1/4,1/4,1/4
   (4,xyz 1/2,0,1/2)
(45) 4* -1/4,y,1/4; -1/4,1/4,1/4
   (4,xyz 0,1/2,1/2)
(46) m x+1/2,y,x
   (m,xyz 1/2,0,1/2)
(47) 4* 0,y; 0,0,0
   (4,xyz 0,0,0)
(48) g (1/4,1/2,1/4) x+1/4,y,x
   (m,xyz 1/2,1/2,0)

Coordinates
(1) t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

Continued}

227.1.1628 Fd3m

(1) x,y,z [u,v,w]
(2) x, y+1/2,z+1/2 [u,v,w]
(3) x+1/2,y+1/2,z [u,v,w]
(4) x+1/2,y,z+1/2 [u,v,w]
(5) z,x,y [w,u,v]
(6) z+1/2,x+1/2,y [w,u,v]
(7) z,x+1/2,y+1/2 [w,u,v]
(8) z+1/2,x+1/2,y [w,u,v]
32  e  .3m  x,x,x [0,0,0]  \bar{x}, \bar{x}+1/2, x+1/2 [0,0,0]

x+1/2,x+1/2,x [0,0,0]  x+1/2, x, x+1/2 [0,0,0]

x+3/4,x+1/4, x+3/4 [0,0,0]  x+1/4, x+1/4, x+1/4 [0,0,0]

x+1/4, x+3/4, x+3/4 [0,0,0]  x+3/4, x+3/4, x+1/4 [0,0,0]

16  d  .\bar{3}m  5/8, 5/8, 5/8 [0,0,0]  3/8, 7/8, 1/8 [0,0,0]  7/8, 1/8, 3/8 [0,0,0]  1/8, 3/8, 7/8 [0,0,0]

16  c  .\bar{3}m  1/8, 1/8, 1/8 [0,0,0]  7/8, 3/8, 5/8 [0,0,0]  3/8, 5/8, 7/8 [0,0,0]  5/8, 7/8, 3/8 [0,0,0]

8   b  \bar{4}3m  1/2, 1/2, 1/2 [0,0,0]  1/4, 3/4, 1/4 [0,0,0]

8   a  \bar{4}3m  0,0,0 [0,0,0]  3/4, 1/4, 3/4 [0,0,0]

### Symmetry of Special Projections

Along [0,0,1]  \quad  p_{\sigma}^\prime 4m'm'

\textbf{a}^* = (a - b)/4  \quad \textbf{b}^* = (a + b)/4

Origin at 1/4,0,z

Along [1,1,1]  \quad  p6'm'm'

\textbf{a}^* = (2a - b - c)/6  \quad \textbf{b}^* = (-a + 2b - c)/6

Origin at x,x,x

Along [1,1,0]  \quad  c2mm1'

\textbf{a}^* = (-a + b)/2  \quad \textbf{b}^* = c

Origin at x,x,1/8
Origin at $\bar{4}3m1'$, at $-1/8,-1/8,-1/8$ from center ($\bar{3}m1'$)

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/8; \quad -1/8 \leq z \leq 1/8; \quad y \leq \min(1/2-x,x); \quad -y \leq z \leq y\]

Vertices

\[0,0,0 \quad 1/2,0,0 \quad 3/8,1/8,1/8 \quad 1/8,1/8,1/8 \quad 3/8,1/8,-1/8 \quad 1/8,1/8,-1/8\]

Symmetry Operations

For \((0,0,0) + \text{set}\)

\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 (0,0,1/2) \quad 0,1/4,z \quad (2z,0,1/2,1/2) \\
(3) & \quad 2 (0,1/2,0) \quad 1/4,y,0 \quad (2z,1/2,1/2,0) \\
(4) & \quad 2 (1/2,0,0) \quad x,0,1/4 \quad (2z,1/2,0,1/2) \\
(5) & \quad 3^* \quad x,x,x \quad (3_{xyz} | 0,0,0) \\
(6) & \quad 3^* \quad (1/3,-1/3,1/3) \quad x+1/6, x+1/6, x \\
(7) & \quad 3^* \quad (-1/3,1/3,1/3) \quad x+1/3, x-1/6, x \\
(8) & \quad 3^* \quad (1/3,1/3,-1/3) \quad x+1/6, x+1/3, x \\
(9) & \quad 3^- \quad x,x,x \quad (3_{xyz}^{-1} | 0,0,0) \\
(10) & \quad 3^- \quad x,x+1/2, x \quad (3_{xyz}^{-1} | 1/2,1/2,0) \\
(11) & \quad 3^- \quad x+1/2, x, x \quad (3_{xyz}^{-1} | 1/2,0,1/2) \\
(12) & \quad 3^- \quad x-1/2, x+1/2, x \quad (3_{xyz}^{-1} | 0,1/2,1/2)
\end{align*}
Continued 227.2.1629  Fd\overline{3}m1'

(33) $\tilde{3}'$  x-1/2,x-1/2,x;
    $\overline{3}'$  x+1/2,x+1/2,x;
    1/8,1/8,5/8
    (3\_\_{xyz}^{-1} 1/4,3/4,3/4)

(37) m  x+1/2,x,z
    (m_{xy} 1/2,1/2,0)

(41) $\overline{4}'$  x,1/4,1/4; 1/4,1/4,1/4
    (4_{x}^{-1} 1/2,1/2,0)

(45) $\overline{4}'$  1/4,y,1/4; 1/4,1/4,1/4
    (4_{y} 1/2,1/2,0)

For (1/2,0,1/2) + set

(1) t  (1/2,0,1/2)
(1/2,0,1/2)

(5) $3'$  (1/3,1/3,1/3)
    x+1/6,x-1/6,x
    1/2,0,1/2
    (3\_\_{xyz}^{-1} 1/2,0,1/2)

(9) $3'$  (1/3,1/3,1/3)
    x-1/6,x+1/6,x
    1/2,0,1/2
    (3\_\_{xyz}^{-1} 1/2,0,1/2)

(13) 2  (1/4,1/4,0)
    x,x,1/8
    (2_{xy} 1/4,1/4,1/4)

(17) $4'$  (1/4,0,0)
    x,1/4,0
    (4_{x}^{-1} 1/4,1/4,1/4)

(21) $\overline{4}'$  (0,1/4,0)
    1/4,y,0
    (4_{y} 1/4,1/4,1/4)

(25) $\overline{1}$  3/8,1/8,3/8
    (1/3,1/8,3/4)

(29) $\overline{3}'$  x-1/2,x-1/2,x;
    1/8,1/8,5/8
    (3\_\_{xyz}^{-1} 3/4,1/4,3/4)

(33) $\tilde{3}'$  x+1/2,x+1/2,x;
    5/8,1/8,1/8
    (3\_\_{xyz}^{-1} 3/4,1/4,3/4)

(37) m  x,x,z
    (m_{xy} 1/2,0,1/2)

(41) $\overline{4}'$  x,0,0; 0,0,0
    (4_{x}^{-1} 0,0,0)

(45) $\overline{4}'$  0,y,0; 0,0,0
    (4_{y} 0,0,0)

Continued 227.2.1629  Fd\overline{3}m1'

(34) $\overline{3}'$  x+1,x-3/2,x;
    1/8,-5/8,7/8
    (3\_\_{xyz} 3/4,1/4,3/4)

(38) g  (1/4,1/4,1/2)
    x+1/4,x,z
    (m_{xy} 1/2,1/2,0)

(42) m  x,y+1/2,y
    (m_{yz} 1/2,1/2,0)

(46) g  (1/4,1/2,-1/4)
    x+1/4,y,x
    (m_{xz} 1/2,1/2,0)
For $(1/2,1/2,0) + \text{set}$

(1) $t (1/2,1/2,0)$
   (1 1/2,1/2,0)

(2) $s (0,0,1/2) 1/4,0,z$
   $(2_s | 1/2,1/2,0)$

(3) $s (0,y,0)$
   $(2_s | 0,0,0)$

(4) $s x,1/4,1/4$
   $(2_s | 0,1/2,1/2)$

(5) $s^* (1/3,1,3/1,3)$
   $x+1/6,x+1/3,x$
   $(3_{xyz}^* | 1,2,1/2,0)$

(6) $s^* x,x+1/2,x$
   $(3_{xyz}^* | 0,1,2,1/2)$

(7) $s^* x+1/2,x-1/2,x$
   $(3_{xyz}^* | 1/2,0,1/2)$

(8) $s^* x,x,x$
   $(3_{xyz}^* | 0,0,0)$

(9) $s^* (1/3,1,3/1,3)$
   $x+1/3,x+1/6,x$
   $(3_{xyz}^* | 1/2,1/2,0)$

(10) $s^* x,x,x$
   $(3_{xyz}^* | 0,0,0)$

(11) $s^* x+1/2,x+1/2,x$
   $(3_{xyz}^* | 1/2,0,1/2)$

(12) $s^* (1,3,1,3,1/3)$
   $x-1/6, x+1/3, x$
   $(3_{xyz}^* | 1/2,0,1/2)$

(13) $s (1/2,1/2,0) x,x+1/4,3/8$
   $(2_s | 1/4,3/4,3/4)$

(14) $s x,x+3/4,1/8$
   $(2_s | 3/4,3/4,1/4)$

(15) $s^* (0,0,3/4) 1/2,-1/4,z$
   $(2_s | 1/4,1/4,1/4)$

(16) $s^* (0,1,1/4) 0,1/4,z$
   $(2_s | 1/4,1/4,1/4)$

(17) $s^* (1/4,0,0) x,3/4,0$
   $(4_{yz}^* | 1/4,3/4,3/4)$

(18) $s x,y+1/2, y$
   $(4_{yz}^* | 1/4,3/4,3/4)$

(19) $s (0,1,4,1/4) 1/8,y,y$
   $(2_s | 3/4,3/4,1/4)$

(20) $s^* (3,4,0,0) x,-1/4,1/2$
   $(2_s | 3/4,3/4,1/4)$

(21) $s^* (0,3,4,0) 1/2,y,1/4$
   $(4_{yz}^* | 1/4,3/4,3/4)$

(22) $s x,1/8,x$
   $(4_{yz}^* | 3/4,1/4,3/4)$

(23) $s^* (0,1,4,0) 0,y,1/4$
   $(4_{yz}^* | 1/4,1/4,1/4)$

(24) $s (1/4,0,-1/4) x+1,3/8,x$
   $(2_s | 3/4,3/4,1/4)$

(25) $s^* (3,8,3,8,1/8)$
   $(2_{xyz} | 1/4,3/4,1/4)$

(26) $d (3/4,1/4,0) x,y,3/8$
   $(m_{xy} | 3/4,1/4,3/4)$

(27) $d (1/4,0,1/4) x,1/8,z$
   $(m_{xy} | 1/4,1/4,1/4)$

(28) $d (0,3/4,3/4) 1/8,y,z$
   $(m_{xy} | 1/4,1/4,3/4)$

(29) $s^* x+1/2,x,x$
   $(5/8,1/8,1/8)$

(30) $s^* x-3/2,x+1,x$
   $(3_{xyz}^* | 3/4,3/4,1/4)$

(31) $s^* x+1/2,x+1,x$
   $(3_{xyz}^* | 1/4,3/4,3/4)$

(32) $s^* x+1/2,x,x$
   $(3_{xyz}^* | 1/4,1/4,3/4)$

(33) $s^* x,x+1/2,x$
   $(1/8,5/8,1/8)$

(34) $s^* x+1/2,x-1/2,x$
   $(3_{xyz}^* | 1/4,1/4,1/4)$

(35) $s^* x-1/2,x+1,x$
   $(3_{xyz}^* | 1/4,1/4,3/4)$

(36) $s^* x+1,x,x$
   $(3_{xyz}^* | 1/4,3/4,3/4)$

(37) $s^* (1,4,1,4/2) x+1/4,x,z$
   $(m_{xz} | 0,1/2,1/2)$

(38) $s (1,2,1/2,0) x,x,z$
   $(m_{xz} | 2,1/2,2,0)$

(39) $s^* (1,4,1,4/2) z,1/4,1/4,1/4$
   $(4_{yz}^* | 1/2,0,1/2)$

(40) $s^* 0,0,0; 0,0,0$
   $(4_{yz}^* | 0,0,0)$

(41) $s^* (0,1/2,0; 0,0,1/2)$
   $(4_{yz}^* | 0,1/2,1/2)$

(42) $s m x,y,y$
   $(m_{yz} | 0,0,0)$

(43) $s m x,y,1/4,y$
   $(m_{yz} | 1/2,1/2,0)$

(44) $s^* x,1/4,1/4,1/4,1/4$
   $(m_{xz} | 1/2,1/2,0)$

(45) $s^* -1/4,y,1/4; -1/4,1/4,1/4$
   $(4_{yz}^* | 1/4,1/4,1/4)$

(46) $s m x+1/2,y,x$
   $(m_{xz} | 1/2,0,1/2)$

(47) $s^* 0,y,0; 0,0,0$
   $(4_{yz}^* | 0,0,0)$

(48) $s (1,4,1/2,1/4) x+1/4,y,x$
   $(m_{xz} | 1/2,1/2,0)$

For $(0,0,0)' + \text{set}$

(1) $1'$
   (1 0,0,0)'

(2) $2'(0,0,1/2) 0,1/4,z$
   $(2_z | 0,1/2,1/2)$

(3) $2'(0,1/2,0) 1/4,y,0$
   $(2_z | 1/2,1/2,0)'$

(4) $2'(1/2,0,0) x,0,1/4$
   $(2_z | 0,1/2,1/2)'$

(5) $s^* ' x,x,x$
   $(3_{xyz} | 0,0,0)'$

(6) $s^* ' (1/3,-1,3/1,3)$
   $x+1/6,x+1/6,x$
   $(3_{xyz} | 1/2,0,1/2)'$

(7) $s^* ' (-1/3,1,3,1/3)$
   $x+1/3,x-1/6,x$
   $(3_{xyz} | 0,1/2,1/2)'$

(8) $s^* ' (1/3,1,3,-1/3)$
   $x+1/6,x+1/3,x$
   $(3_{xyz} | 0,1/2,1/2)'$

(9) $s^* ' x,x,x$
   $(3_{xyz} | 0,0,0)'$

(10) $s^* ' x,x+1/2,x$
    $(3_{xyz} | 1/2,0,1/2)'$

(11) $s^* ' x+1/2,x,x$
    $(3_{xyz} | 1/2,0,1/2)'$

(12) $s^* ' x-1/2,x+1/2,x$
    $(3_{xyz} | 0,1/2,1/2)'$

(13) $2'(1/2,1/2,0) x,x-1/4,3/8$
    $(2_s | 1/4,1/4,1/4,3/4)'$

(14) $2'(x,x+1/4,1/8$
    $(2_s | 1/4,1/4,1/4,1/4)'$

(15) $s^* ' (0,0,3/4) 1/2,1/4,z$
    $(4_{yz}^* | 1/4,3/4,3/4)'$

(16) $s^* ' (0,0,1/4) 0,3/4,z$
    $(4_{yz}^* | 3/4,3/4,1/4)'$
Continued 227.2.1629  Fd3m1'

(37) m' x+1/2, x, z  (38) g' (1/4,1/4,1/2)  x-1/4,x,z  (39) 3- ' 0,0,0; z, 0,0,0  (40) 4- ' 1/4,-1/4,z; 1/4,-1/4,1/4  
( m_y, 1/2,1/2,0')  (m_x, 0,1/2,1/2,0')  (4-z, 0,0,0,0')  (4-z', 1/2,0,1/2,0')

(41) 4- ' x,1/4,1/4; 1/4,1,1/4,1/4  (42) g' (1/2,-1/4,1/4)  x,y+1/4, y  (43) g' (0,1/2,1/2)  x,y,y  (44) 4- ' x,0,0; 0,0,0  
(4-z, 1/2,0,1/2,0')  (m_yz, 1/2,0,1/2,0')  (m_yz, 0,1/2,1/2,0')  (4-z, 0,0,0,0')

(45) 4- ' 1/4,y,1/4; 1/4,1,1/4,1/4  (46) m'  x,y,x  (47) 4- ' 1/2,y,0; 1/2,0,0  (48) g' (1/4,1/2,1/4)  x-1/4,y,x  
(4-z, 1/2,0,1/2,0')  (m_xz, 0,0,0,0')  (4-z, 1/2,0,1/2,0')

For (1/2,0,1/2)' + set

(1) t' (1/2,0,1/2)  (2) 2' 1/4,1/4,z  (3) 2' (0,1/2,0) 0,y,1/4  (4) 2' x,0,0  
(1/2,0,1/2)'  (2/2,1/2,0,0)'  (2/2,0,1/2,1/2,0)'  (2/2,0,1/2,1/2,0)'  (2/2,0,1/2,1/2,0)'

(5) 3+ ' (1/3,1/3,1/3)  x+1/6,x-1/6,x  (6) 3' x,x,x  (7) 3' x+1/2,x,x  (8) 3' x+1/2,x,x  
(x,1/2,0,1/2)'  (m_xz, 1/2,0,1/2,0')  (3_xz, 1/2,0,1/2,0')  (3_xz, 1/2,0,1/2,0')  (3_xz, 1/2,0,1/2,0)'

(9) 3+ ' (1/3,1/3,1/3)  x+1/6,x-1/6,x  (10) 3' (-1/3,1/3,1/3)  x+1/6,x+1/6,x  (11) 3' x,x,x  (12) 3' x,x+1/2,x  
(3_xz, 1/2,0,1/2,0')  (3_xz, 1/2,0,1/2,0')  (3_xz, 0,1/2,2/1,0')  (3_xz, 0,1/2,2/1,0')  (3_xz, 0,1/2,2/1,0)'

(13) 2' (1/4,1/4,0)  x,x,1/8  (14) 2' (1/4,1/4,0)  x,x+1/2,3/8  (15) 4' (0,0,1/4) 3/4,0,z  (16) 4' (0,0,3/4) -1/4,1,2,3  
(2/2,1/4,1/4,1/4)'  (2/2,1/4,1/4,1/4)'  (4_z, 3/4,1/4,3/4)'  (4_z, 1/4,3/4,3/4)'  (4_z, 1/4,3/4,3/4)'

(17) 4' (1/4,0,0)  x,1/4,0  (18) 2' (0,3/4,3/4) 1/8,y,y  (19) 2' (0,-1/4,1/4) 3/8,y+1/2,y  (20) 4' (3/4,0,0) x,1/4,1/2  
(4_z, 1/4,1/4,1/4)'  (2/2,1/4,1/4,1/4)'  (2/2,1/4,1/4,1/4)'  (2/2,1/4,1/4,1/4)'  (2/2,1/4,1/4,1/4)'

(21) 4' (0,1/4,0) 1/4,y,0  (22) 2' (1/2,0,1/2) x+1/4,3/8,x  (23) 4' (0,3/4,0) -1/4,y,y,1/2  (24) 2' x+3/4,1/8,x  
(4_z, 1/4,1/4,1/4)'  (2/2,1/4,1/4,1/4)'  (4_z, 1/4,3/4,3/4)'  (4_z, 1/4,3/4,3/4)'

(25) 1- 3/8,1/8,3/8  (26) d' (3/4,3/4,0) x,1/8,1/8  (27) d' (1/4,0,3/4) 3/4,1/4,3/4  (28) d' (0,1/4,1/4) 1/8,y,z  
(3, 3/4,1/4,3/4)'  (m_xz, 3/4,1/4,3/4)  (m_xz, 1/4,3/4,3/4)  (m_xz, 1/4,3/4,3/4)  (m_xz, 1/4,3/4,3/4)'

(29) 3' x-1/2-x-1/2,x; 1/8,1/8,5/8  (30) 3' x-1/2,x+1/2,x; -1/8,1/8,3/8  (31) 3' x-1/2,x+3/2,x; 1/8,8,5/8  (32) 3' x+3/2, x+1/2,x; 1/8,8,5/8  
(3_xz, 3/4,1/4,3/4)'  (3_xz, 3/4,1/4,3/4)'  (3_xz, 3/4,1/4,3/4)'  (3_xz, 1/4,3/4,1/4)'  (3_xz, 3/4,3/4,3/4)'

(33) 3' x+1/2,x,x; 5/8,1/8,1/8  (34) 3' x+1/2, x-1, x; 1/8,-1/8,7/8  (35) 3' x+1/2, x-1, x; 1/8,-1/8,7/8  (36) 3' x+3/2, x-1, x; 7/8,1/8,5/8  
(3_xz, 3/4,1/4,3/4)'  (3_xz, 1/4,3/4,1/4)'  (3_xz, 1/4,3/4,1/4)'  (3_xz, 1/4,3/4,1/4)'  (3_xz, 3/4,3/4,3/4)'

(37) m' x, x, z  (38) g' (1/4,1/4,1/2) x+1/4,x,z  (39) 3- ' 0,1/2,z; 0,1/2,0  (40) 4- ' 1/4,1/4,z; 1/4,1/4,1/4  
( m_y, 0,0,0,0')  (m_xz, 1/2,0,1/2,0')  (m_xz, 0,1/2,0,1/2,0')  (4_z, 0,1/2,1/2,0')

(41) 4- ' x,0,0; 0,0,0  (42) m' x,y+1/2,y  (43) g' (1/2,1/4,1/4) x,y-1/4,y  (44) 4- ' x,1/4,-1/4; 1/4,1/4,1/4  
(4-z, 0,0,0,0')  (m_yz, 1/2,0,1/2,0')  (m_yz, 1/2,0,1/2,0')  (4-z, 1/2,0,1/2,0')

(45) 4- ' 0, y,0; 0,0,0  (46) g' (1/4,1/2,-1/4) x+1/4,y,x  (47) 4- ' 1/4,y, y; 1/4,1/4,1/4  (48) g' (1/2,0,1/2) x,y,x  
(4-z, 0,0,0,0')  (m_xz, 1/2,0,1/2,0')  (m_xz, 1/2,0,1/2,0') (m_xz, 1/2,0,1/2,0)'

For (1/2,1/2,0)'+ set

(1) t' (1/2,1/2,0)  (2) 2' (0,0,1/2) 1/4,0,z  (3) 2' 0,y,0  (4) 2' x,1/4,1/4  
(1/2,1/2,0)'  (1/2,0,1/2,0)'  (2,0,1/2,0)'  (2,0,1/2,0)'  (2,0,1/2,0)'

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(5) $3^\ast$ $(1/3,1/3,1/3)$

$x+1/6, x+1/3, x$

$(3_{xyz} \ 1/2,1/2,0)'$

(6) $3^\ast$ \(x, x+1/2, x\)

(7) $3^\ast$ \(x+1/2, x-1/2, x\)

(8) $3^\ast$ \(x, x, x\)

Positions

Continued 227.2.1629 Fd3m1'  

Generators selected 

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25); 1'.

Full list of Wyckoff positions

Continued
Continued

<table>
<thead>
<tr>
<th>16</th>
<th>d</th>
<th>$\bar{3}m1'$</th>
<th>5/8,5/8,5/8 [0,0,0]</th>
<th>3/8,7/8,1/8 [0,0,0]</th>
<th>7/8,1/8,3/8 [0,0,0]</th>
<th>1/8,3/8,7/8 [0,0,0]</th>
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<td>16</td>
<td>c</td>
<td>$\bar{3}m1'$</td>
<td>1/8,1/8,1/8 [0,0,0]</td>
<td>7/8,3/8,5/8 [0,0,0]</td>
<td>3/8,5/8,7/8 [0,0,0]</td>
<td>5/8,7/8,3/8 [0,0,0]</td>
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<tr>
<td>8</td>
<td>b</td>
<td>$4\bar{3}m1'$</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>a</td>
<td>$4\bar{3}m1'$</td>
<td>0,0,0 [0,0,0]</td>
<td>3/4,1/4,3/4 [0,0,0]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm1'

$\text{a}^* = (\text{a} - \text{b})/4$  $\text{b}^* = (\text{a} + \text{b})/4$

Origin at 0,0,z

Along [1,1,1] p6mm1'

$\text{a}^* = (2\text{a} - \text{b} - \text{c})/6$  $\text{b}^* = (-\text{a} + 2\text{b} - \text{c})/6$

Origin at x,x,x

Along [1,1,0] c2mm1'

$\text{a}^* = (-\text{a} + \text{b})/2$  $\text{b}^* = \text{c}$

Origin at x,x,1/8
Fd'3'm

227.3.1630

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0
(10) 3' x,x+1/2,x
(3_{xyz}^{-1}|0,0,0)
(11) 3' x+1/2,x,x
(3_{xyz}|1/2,0,1/2)
(12) 3' x-1/2,x+1/2,x
(3_{xyz}|0,1/2,1/2)

(2) 2 (0,0,1/2) 0,1/4,z
(2) 1/2,0,1/2,0
(2) y+1/6,x+1/6,x
(2) x+1/3, x-1/6,x
(2) x+1/6, x+1/3,x
(2) x+1/3, x-1/2, 1/2
(2) x+1/2, 1/2,0

(3) 2 (0,1/2,0) 1/4,y,0
(3) 1/2,1/2,0,y
(3) x+1/6, x+1/3, x
(3) x+1/3, x-1/2, 1/2
(3) x+1/2, 1/2,0

(4) 2 (1/2,0,0) x,0,1/4
(4) 1/2,0,1/2

(5) 3' x,x,x
(5) 0,0,0
(5) x+1/6, x+1/6,x
(5) x+1/3, x-1/6,x
(5) x+1/6, x+1/3,x
(5) x+1/3, x-1/2, 1/2
(5) x+1/2, 1/2,0

(6) 3' (1/3,-1/3,1/3)
(6) x+1/6,x+1/6,x
(6) x+1/3, x-1/6,x
(6) x+1/6, x+1/3,x
(6) x+1/3, x-1/2, 1/2
(6) x+1/2, 1/2,0

(7) 3' (-1/3,1/3,1/3)
(7) x+1/6,x+1/6,x
(7) x+1/3, x-1/6,x
(7) x+1/6, x+1/3,x
(7) x+1/3, x-1/2, 1/2
(7) x+1/2, 1/2,0

(8) 3' (1/3,1/3,-1/3)
(8) x+1/6,x+1/6,x
(8) x+1/3, x-1/6,x
(8) x+1/6, x+1/3,x
(8) x+1/3, x-1/2, 1/2
(8) x+1/2, 1/2,0

(9) 3' x,x,x
(9) 0,0,0
(9) x+1/6, x+1/6,x
(9) x+1/3, x-1/6,x
(9) x+1/6, x+1/3,x
(9) x+1/3, x-1/2, 1/2
(9) x+1/2, 1/2,0

(3_{xyz}^{-1}|0,0,0)
(3_{xyz}|1/2,1/2,0)
(3_{xyz}^{-1}|1/2,1/2,0)

(3_{xyz}^{-1}|0,0,0)
(3_{xyz}|1/2,0,1/2)
(3_{xyz}^{-1}|0,1/2,1/2)

Origin at 43m, at -1/8,-1/8,-1/8 from center (3'm)

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/8; -1/8 ≤ z ≤ 1/8; y ≤ min(1/2-x,x);
-y ≤ z ≤ y

Vertices
0,0,0 1/2,0,0 3/8,1/8,1/8 1/8,1/8,1/8 3/8,1/8,-1/8 1/8,1/8,-1/8 1/8,1/8,-1/8

Symmetry Operations

For (0,0,0) + set

(1) 1
(1) 0,0,0
(10) 3' x,x+1/2,x
(3_{xyz}^{-1}|0,0,0)
(11) 3' x+1/2,x,x
(3_{xyz}^{-1}|1/2,0,1/2)
(12) 3' x-1/2,x+1/2,x
(3_{xyz}^{-1}|0,1/2,1/2)

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(33) $\overline{3}'\cdot x-1/2, x-1/2,$
$sym\; x-1/2, x-1/2,$
$1/8, 1/8, 5/8$
$(\overline{3}_{xyz}\; 1/4, 1/4, 1/4')$

(37) $m\; x+1/2, \overline{x}, z$
$(m_{xyz}\; 1/2, 1/2, 0)$

(41) $\overline{4}\cdot x, 1/4, 1/4,$
$sym\; x, 1/4, 1/4,$
$1/2, 0, 1/2$
$(\overline{4}_{x}\; 1/2, 1/2, 0)$

(45) $\overline{4}\cdot 1/4, y, 1/4,$
$sym\; 1/4, y, 1/4,$
$1/2, 1/2, 0$
$(\overline{4}_{y}\; 1/2, 1/2, 0)$

$\overline{3}'\cdot x+1/2, x+1/2,$
$sym\; x+1/2, x+1/2,$
$1/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4')$

(38) $g\; (1/4, 1/4, 1/2)$
$(m_{xy}\; 0, 1/2, 1/2)$

(42) $g\; (1/2, -1/4, 1/4)$
$(m_{yz}\; 0, 1/2, 1/2)$

(46) $g\; (1/4, 1/2, -1/4)$
$(m_{xz}\; 1/2, 1/2, 0)$

(47) $\overline{4}\cdot 1/2, y, 0,$
$sym\; 1/2, y, 0,$
$1/2, 0, 0$
$(\overline{4}_{y}\; 1/2, 0, 1/2)$

$\overline{3}'\cdot x+1/2, x+1/2,$
$sym\; x+1/2, x+1/2,$
$1/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4')$

(39) $4\cdot 0, 0, z,$
$sym\; 0, 0, z,$
$0, 0, 0$
$(4_{z}\; 0, 0, 0)$

(43) $g\; (0, 1/2, 1/2)$
$(m_{yz}\; 0, 1/2, 1/2)$

$\overline{4}\cdot x, 0, 0,$
$sym\; x, 0, 0,$
$0, 0, 0$
$(\overline{4}_{x}\; 0, 0, 0)$

$\overline{3}'\cdot x+1/2, x+1/2,$
$sym\; x+1/2, x+1/2,$
$1/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 1/4, 1/4, 1/4')$

(48) $g\; (1/4, 1/2, 1/4)$
$(m_{xz}\; 0, 1/2, 1/2)$

For $(1/2, 0, 1/2) +$ set

(1) $(1/2, 0, 1/2)$

(2) $(1/2, 1/2, 0)$

(3) $(0, 1/2, 0)$

(4) $(1/2, 0, 0)$

(5) $3'$
$sym\; x, x, x,$
$1/4, 1/4, 1/4$
$x+1/6, x+1/6,$
$(3_{xyz}\; 1/2, 0, 1/2)$

(9) $3'$
$sym\; x, x, x,$
$1/4, 1/4, 1/4$
$x+1/6, x+1/6,$
$(3_{xyz}\; 1/2, 0, 1/2)$

(13) $2'$
$sym\; x, x, x,$
$1/4, 1/4, 1/4$
$(2_{xy}\; 1/4, 1/4, 1/4')$

(14) $2'$
$sym\; x, x, x,$
$1/4, 1/4, 3/8$
$(2_{xy}\; 1/4, 1/4, 1/4)$

(18) $2'$
$sym\; x, x, x,$
$0, 3/4, 3/4$
$(2_{yz}\; 1/4, 1/4, 1/4)$

(19) $2'$
$sym\; x, x, x,$
$0, 3/4, 3/4$
$(2_{yz}\; 1/4, 1/4, 1/4)$

(22) $2'$
$sym\; x, x, x,$
$0, 3/4, 3/4$
$(2_{xy}\; 1/4, 1/4, 1/4)$

(26) $d$'$
$sym\; x, x, x,$
$3/4, 3/4, 3/4$
$(d_{xyz}\; 3/4, 3/4, 3/4')$

(27) $d$'$
$sym\; x, x, x,$
$3/4, 3/4, 3/4$
$(d_{xyz}\; 3/4, 3/4, 3/4')$

(30) $3'$
$sym\; x, x, x,$
$1/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4)$

(31) $\overline{3}'\;
$sym\; x, x, x,$
$1/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4')$

(32) $\overline{3}'\;
$sym\; x, x, x,$
$1/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4)$

(33) $\overline{3}'\;
$sym\; x, x, x,$
$5/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4)$

(35) $\overline{3}'\;
$sym\; x, x, x,$
$5/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4)$

(36) $\overline{3}'\;
$sym\; x, x, x,$
$5/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4)$

(37) $m\; x, x, z$
$(m_{xyz}\; 0, 0, 0)$

(40) $4'$
$sym\; x, x, x,$
$1/4, 1/4, 1/4$
$(4_{x}\; 1/2, 1/2, 0)$

(41) $4'$
$sym\; x, x, x,$
$0, 0, 0$
$(4_{y}\; 0, 0, 0)$

(42) $m\; x, y, 1/2,$
$(m_{yz}\; 0, 1/2, 1/2)$

(43) $g\; (1/2, 1/4, 1/4)$
$(m_{yz}\; 1/2, 0, 1/2)$

(44) $4'$
$sym\; x, x, x,$
$1/4, 1/4, 1/4$
$(4_{x}\; 1/2, 1/2, 0)$

(45) $4'$
$sym\; x, x, x,$
$0, 0, 0$
$(4_{y}\; 0, 0, 0)$

$\overline{3}'\cdot x+1/2, x+1/2,$
$sym\; x+1/2, x+1/2,$
$1/8, 1/8, 1/8$
$(\overline{3}_{xyz}\; 3/4, 1/4, 1/4)$

(39) $4\cdot 0, 1/2, z,$
$sym\; 0, 1/2, z,$
$0, 1/2, 0$
$(4_{z}\; 1/2, 1/2, 0)$

(43) $g\; (1/2, 1/4, 1/4)$
$(m_{yz}\; 1/2, 0, 1/2)$

(47) $\overline{4}\cdot 1/4, y, 1/4,$
$sym\; 1/4, y, 1/4,$
$1/4, 1/4, 1/4$
$(\overline{4}_{y}\; 1/4, 1/4, 1/4)$

(48) $g\; (1/2, 0, 1/2)$
$(m_{xz}\; 1/2, 0, 1/2)$
For (1/2, 1/2, 0) + set

(1) t (1/2, 1/2, 0)
(1) t (1/2, 1/2, 0)

(5) 3' (1/3, 1/3, 1/3)
(5) 3' (1/3, 1/3, 1/3)

(9) 3' (1/3, 1/3, 1/3)
(9) 3' (1/3, 1/3, 1/3)

(13) 2' (1/2, 1/2, 0)
(13) 2' (1/2, 1/2, 0)

(17) 4' (1/4, 0, 0)
(17) 4' (1/4, 0, 0)

(21) 4' (0, 3/4, 0)
(21) 4' (0, 3/4, 0)

(25) 1' (3/8, 3/8, 1/8)
(25) 1' (3/8, 3/8, 1/8)

(29) 3' x+1/2, x; x, x (m_y x+1/2, x)
(29) 3' x+1/2, x; x, x (m_y x+1/2, x)

(33) 3' x, x+1/2, x; 1/8, 5/8, 1/8
(33) 3' x, x+1/2, x; 1/8, 5/8, 1/8

(37) g (-1/4, 1/4, 1/2)
(37) g (-1/4, 1/4, 1/2)

(41) 4' (0, 1/2, 0; 0, 0, 1/2
(41) 4' (0, 1/2, 0; 0, 0, 1/2

(45) 4' -1/4, y, 1/4; -1/4, 1/4, 1/4
(45) 4' -1/4, y, 1/4; -1/4, 1/4, 1/4

Generators selected
(1); t(1, 0, 0); t(0, 1, 0); t(0, 1/2, 1/2); t(1, 2/0, 1/2); (2); (3); (5); (13); (25).

Positions
Multplicity, Wyckoff letter, Site Symmetry.

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(1) x, y, z [u, v, w]
(6) z+1/2, x, y+1/2 [w, u, v]

(2) x, y+1/2, z+1/2 [u, v, w]
(7) z, x+1/2, y+1/2 [w, u, v]

(3) x+1/2, y+1/2, z [u, v, w]
(8) z+1/2, x+1/2, y [w, u, v]

(4) x, y+1/2, z+1/2 [u, v, w]
(9) 3- (1/3, -1/3, 1/3)

(10) x, x, x
(11) x+1/2, x+1/2, x

(12) x+1/2, x+1/2, x
(13) 2' (1/2, 1/2, 0)
(14) 2' x, x+3/4, 1/8
(15) 4' 0, 0, 3/4 1/2, -1/4, z
(16) 4' 0, 0, 1/4 0, 1/4, z

(17) 4' (1/4, 0, 0)
(18) 2' 0, 1/4, 1/4; 1/8, y, y
(19) 2' 0, 1/4, 1/4; 1/8, y, y
(20) 4' (3/4, 0, 0)
(21) 4' (0, 3/4, 0)
(22) 2' (3/4, 0, 3/4)
(23) 4' 0, 1/4, 0
(24) 2' (1/4, 0, -1/4)

(25) 1' (3/8, 3/8, 1/8)
(26) d' (3/4, 1/4, 0)
(27) d' 1/4, 0, 1/4
(28) d' 0, 3/4, 3/4

(29) 3' x+1/2, x; 5/8, 1/8
(30) 3' x+1/2, x; 5/8, 1/8
(31) 3' x+1/2, x+1, x; 5/8, 7/8, 1/8
(32) 3' x+1/2, x; 3/8, 1/8, 1/8

(33) 3' x, x+1/2, x; 1/8, 5/8, 1/8
(34) 3' x+1/2, x; 1/8, 5/8, 1/8
(35) 3' x+1/2, x+1, x; 5/8, 7/8, 1/8
(36) 3' x+1/2, x; 7/8, 1/8, 1/8

(37) g (-1/4, 1/4, 1/2) x+1/4, x, z
(38) g (1/2, 1/2, 0) x, x, z
(39) 4' 1, 1/4, 1/4, z; 1/4, 1/4, 1/4
(40) 4' 0, 0, z; 0, 0, 0

(41) 4' x, 0, 1/2; 0, 0, 1/2
(42) m x, y, y
(43) g (1/2, 1/4, 1/4) x, y+1, y+1, y+1, y+1
(44) 4' x, 1/4, 1/4, 1/4

(45) 4' -1/4, y, 1/4; -1/4, 1/4, 1/4
(46) m x+1/2, y, x
(47) 4' 0, 0, 0
(48) g (1/4, 1/2, 1/4)

227.3.1630 - 4 - 3807
Symmetry of Special Projections

<table>
<thead>
<tr>
<th>32 e</th>
<th>.3m</th>
<th>x,x,x [0,0,0]</th>
<th>x,x+1/2,x+1/2 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>x+1/2,x+1/2,x [0,0,0]</td>
<td>x+1/2,x,x+1/2 [0,0,0]</td>
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<tr>
<td></td>
<td></td>
<td>x+3/4,x+1/4,x+3/4 [0,0,0]</td>
<td>x+1/4,x+1/4,x+1/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>x+1/4,x+3/4,x+3/4 [0,0,0]</td>
<td>x+3/4,x+3/4,x+1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

| 16 d  | .3' m | 5/8,5/8,5/8 [0,0,0] | 7/8,1/8,3/8 [0,0,0] | 1/8,3/8,7/8 [0,0,0] |
| 16 c  | .3' m | 1/8,1/8,1/8 [0,0,0] | 7/8,3/8,5/8 [0,0,0] | 5/8,7/8,3/8 [0,0,0] |
| 8 b   | 43m  | 1/2,1/2,1/2 [0,0,0] | 1/4,3/4,1/4 [0,0,0] |
| 8 a   | 43m  | 0,0,0 [0,0,0] | 3/4,1/4,3/4 [0,0,0] |

**Symmetry of Special Projections**

Along [0,0,1]  
\( a^* = (a - b)/4 \)  
\( b^* = (a + b)/4 \)
Origin at 0,0,z

Along [1,1,1]  
\( a^* = (2a - b - c)/6 \)  
\( b^* = (-a + 2b - c)/6 \)
Origin at x,x,x

Along [1,1,0]  
\( a^* = c \)  
\( b^* = -(a + b)/2 \)
Origin at x,x,1/8
Origin at 4'3m', at -1/8,-1/8,-1/8 from center (3m')

Asymmetric unit  
\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/8; \quad -1/8 \leq z \leq 1/8; \quad y \leq \min(1/2-x,x); \quad -y \leq z \leq y\]

Vertices  
\[0,0,0 \quad 1/2,0,0 \quad 3/8,1/8,1/8 \quad 1/8,1/8,1/8 \quad 3/8,1/8,-1/8 \quad 1/8,1/8,-1/8\]

Symmetry Operations  
For \((0,0,0) + \) set

1. \((1) 1\)  
   \(\begin{pmatrix} 1 \\ 0,0,0 \end{pmatrix}\)

2. \((2) 2\)  
   \(\begin{pmatrix} 0,0,1/2 \\ 1/4,z \end{pmatrix}\)

3. \((3) 2\)  
   \(\begin{pmatrix} 0,1/2,0 \\ 1/4,y,0 \end{pmatrix}\)

4. \((4) 2\)  
   \(\begin{pmatrix} 1/2,0,0 \\ x,0,1/4 \end{pmatrix}\)

5. \((5) 3^+\)  
   \(\begin{pmatrix} x,x,x \end{pmatrix}\)

6. \((6) 3^+\)  
   \(\begin{pmatrix} 1/3,-1/3,1/3 \\ x+1/6, x+1/6, x \end{pmatrix}\)

7. \((7) 3^+\)  
   \(\begin{pmatrix} 1/3,1/3,1/3 \\ x+1/3, x-1/6, x \end{pmatrix}\)

8. \((8) 3^+\)  
   \(\begin{pmatrix} 1/3,1/3,-1/3 \\ x+1/6, x+1/3, x \end{pmatrix}\)

9. \((9) 3^-\)  
   \(\begin{pmatrix} x,x,x \end{pmatrix}\)

10. \((10) 3^-\)  
    \(\begin{pmatrix} x,x+1/2, x \end{pmatrix}\)

11. \((11) 3^-\)  
    \(\begin{pmatrix} +1/2, x, x \end{pmatrix}\)

12. \((12) 3^-\)  
    \(\begin{pmatrix} x-1/2, x+1/2, x \end{pmatrix}\)
Continued

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(2) 2 (0,0,1/2) 1/4,0,z
(3) 2 (0,y,0) (2z) (2,0,1/2)
(4) 2 x,1/4,1/4 (2z) (0,1/2,1/2)
(5) 3* (1/3,1/3,1/3) x+1/6,x+1/3,x
(3xyz) (1/2,1/2,0)
(6) 3* x,x+1/2,x
(7) 3* x+1/2,x-1/2,x
(8) 3* x,x,x
(9) 3' (1/3,1/3,1/3) x+1/3,x+1/6,x
(3xyz) (1/2,1/2,0)
(10) 3' x,x,x
(11) 3' x+1/2,x+1/2,x
(12) 3' (1/3,-1/3,1/3) x-1/6,x+1/3,x
(13) 2' (1/2,1/2,0) x,x+1/4,3/8
(2xyz) (1/4,3/4,3/4)' (2) 2 x, x+3/4,1/8
(2xyz) (3,1/4,1/4,1/4)' (15) 4* (0,0,3/4) 1/2,-1/4, z
(4z) (2) 1/4,1/4,1/4)' (16) 4* (0,1/4,0) 0,1/4, z
(4z) (2) 1/4,1/4,1/4)' (17) 4* (1/4,0,0) x,3/4,0
(4z) (1/4,3/4,3/4)' (19) 2' (0,1/4,-1/4) 3/8,y+1/2, y
(2xyz) (3,1/4,1/4,1/4)' (20) 4* (3/4,0,0) x,-1/4,1/2
(4z) (3,1/4,1/4,1/4)' (18) 2' (0,1/4,1/4) 1/8,y,y
(2xyz) (3,1/4,1/4,1/4)' (21) 4* (0,3/4,0) 1/2,y,1/4
(4z) (1/4,3/4,3/4)' (22) 2' (3/4,0,3/4) x,1/8,x
(2xyz) (3,1/4,1/4,1/4)' (23) 4' (0,1/4,0) 0,y,1/4
(4z) (1/4,1/4,1/4)' (24) 2' (1/4,0,-1/4) x+1/2,3/8,x
(2xyz) (3,1/4,1/4,1/4)' (25) 1/2 3/4,3/4,1/8
(3,1/4,1/4,1/4) (26) d (3/4,1,1/4) x,y,3/8
(3xyz) (3,1/4,1/4,1/4) (27) d (1/4,0,1/4) x,1/8,z
(3xyz) (3,1/4,1/4,1/4) (28) d (0,3/4,3/4) 1/8,y,z
(3xyz) (3,1/4,1/4,1/4) (29) 3* x+1/2,x,x;
(3xyz) (5,1/8,1/8) (31) 3* x+1/2,x+1, x;
(3xyz) (3,1/4,3/4,1/4) (32) 3* x+1/2,x; x;
(3xyz) (3,1/4,3/4,1/4) (33) 3* x,x+1/2,x;
(3xyz) (5,1/8,1/8) (35) 3* x-1/2,x+1, x;
(3xyz) (3,1/4,3/4,1/4) (36) 3* x+1, x;
(3xyz) (3,1/4,3/4,1/4) (37) g' (-1/4,1/4,1/2) x+1/4,x,z
(mxyz) (0,1/2,1/2)' (38) g' (1/2,1/2,0) x,x,x
(mxyz) (1/2,1/2,0)' (39) 4* 1/4,1/4,z; 1/4,1/4,1/4
(4z) (1/2,0,1/2)' (40) 4* 0,0,0; 0,0,0
(4z) (1/2,0,1/2)' (41) 4' x,0,1/2; 0,0,1/2
(4z) (0,1/2,1/2)' (42) m' x,y,y
(mxyz) (0,0,0)' (43) g' (1/2,1/4,1/4) x,y+1/4,y
(mxyz) (1/2,1/2,0)' (44) 4' x,1/4,1/4; 1/4,1/4,1/4
(4z) (1/2,0,1/2)' (45) 4' x,-1/4,y,1/4; -1/4,1,4,1/4
(4z) (0,1/2,1/2)' (46) m' x+1/2,y,x
(mxyz) (1/2,0,1/2)' (47) 4' y,0; 0,0,0
(4z) (0,0,0)' (48) m' x+1/2,y,x
(mxyz) (1/2,0,1/2)' (49) 4' y,0; 0,0,0
(4z) (0,0,0)' (49) 4' y,0; 0,0,0

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.
192 i 1

(1) x,y,z [u,v,w]
(2) x, y+1/2,z+1/2 [u,v,w]
(3) x+1/2,y+1/2,z [u,v,w]
(4) x+1/2,y+z+1/2 [u,v,w]
(5) x+1/2,y,z+1/2 [w,u,v]
(6) z+1/2,x+1/2 [w,u,v]
(7) z, x+1/2,y+1/2 [w,u,v]
(8) z+1/2,x+1/2, y [w,u,v]
Symmetry of Special Projections

Along $[0,0,1]$  $p4mm'$
\[ \mathbf{a}^* = (\mathbf{a} - \mathbf{b})/4 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/4 \]
Origin at $0,0,z$

Along $[1,1,1]$  $p6mm'$
\[ \mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/6 \quad \mathbf{b}^* = (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/6 \]
Origin at $x,x,x$

Along $[1,1,0]$  $c2mm'$
\[ \mathbf{a}^* = \mathbf{c} \quad \mathbf{b}^* = -(\mathbf{a} + \mathbf{b})/2 \]
Origin at $x,x,1/8$
Origin at \( \bar{4}3m' \), at \(-1/8, -1/8, -1/8\) from center \( (3m')\)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/8; \quad -1/8 \leq z \leq 1/8; \quad y \leq \min(1/2-x,x); \quad -y \leq z \leq y \]

Vertices

\[ 0,0,0 \quad 1/2,0,0 \quad 3/8,1/8,1/8 \quad 1/8,1/8,1/8 \quad 3/8,1/8,-1/8 \quad 1/8,1/8,-1/8 \]

Symmetry Operations

For \((0,0,0)\) set

\[
\begin{align*}
(1) & \quad 1 \\
(1) & \quad 0,0,0 \\
(5) & \quad x,x,x \\
(3_{xyz} | 0,0,0) & \\
(9) & \quad x,x,x \\
(3_{xyz}^{-1}| 0,0,0) & \\
(2) & \quad 2 (0,0,1/2) \quad 0,1/4,z \\
& \quad (2\bar{1}) 0,1/2,1/2 \\
(6) & \quad 3^{-} (1/3,-1/3,1/3) \\
& \quad x+1/6,x+1/6,x \\
& \quad (3_{xyz}^{-1}| 1/2,0,1/2) \\
(10) & \quad 3^{-} x, x+1/2,x \\
& \quad (3_{xyz}^{-1}| 1/2,1/2,0) \\
(12) & \quad 3^{-} x, x+1/2,x \\
& \quad (3_{xyz}^{-1}| 0,1/2,1/2) \\
(3) & \quad 2 (0,1/2,0) \quad 1/4,y,0 \\
& \quad (2\bar{1} 1/2,1/2,0) \\
(7) & \quad 3^{-} (-1/3,1/3,1/3) \\
& \quad x+1/3,x-1/6,x \\
& \quad (3_{xyz}^{-1}| 0,1/2,1/2) \\
(11) & \quad 3^{-} \bar{x}, \bar{x}+1/2,\bar{x} \\
& \quad (3_{xyz}^{-1}| 1/2,0,1/2) \\
(8) & \quad 3^{-} (1/3,1/3,-1/3) \\
& \quad x+1/6,x+1/3,x \\
& \quad (3_{xyz}^{-1}| 1/2,1/2,0) \\
(4) & \quad 2 (1/2,0,0) \quad x,0,1/4 \\
& \quad (2\bar{1} 1/2,0,1/2) \\
(11) & \quad 3^{-} \bar{x}, \bar{x}+1/2,\bar{x} \\
& \quad (3_{xyz}^{-1}| 1/2,0,1/2) \\
\end{align*}
\]
For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)  
(1) 1/2,1/2,0

(2) 2 (0,0,1/2) 1/4,0,z  
(2) 0,0,1/2

(3) 2 0,y,0  
(3) 0,0,0

(4) 2 x,1/4,1/4  
(4) 0,1/2,1/4

(5) 3' (1/3,1/3,1/3)  
(3) 1/3,1/3,1/3

x+1/6,x+1/3,x  
(3) x

(3) x+1/2,x+1/2  
(3) x

(7) 3' x+1/2,x-1/2  
(7) x

(8) 3' x,x,x  
(8) x

(9) 3' (1/3,1/3,1/3)  
(9) 1/3,1/3,1/3

x+1/6,x+1/3,x  
(3) x

(3) x  
(3) x

(11) 3' x+1/2,x+1/2,x  
(11) x

(12) 3' (1/3,1/3,1/3)  
(12) x-1/6,x+1/3,x  

(3) x+1/2,x+1/2  
(3) x

(13) 2 (1/2,1/2,0)  
(13) 1/2,1/2,0

x,x+1/4,3/8  
(3) x

(14) 2 x,x+3/4,1/8  
(14) x

(15) 4' (0,0,3/4) 1/2,-1/4,z  
(15) x

(16) 4* (0,0,1/4) 0,1/4,z  
(16) x

(17) 4' (1/4,0,0) x,3/4,0  
(17) x

(18) 2 (0,1/4,1/4) 1/8,y,y  
(18) x

(19) 2 (0,1/4,-1/4) 3/8,y+1/2,y  
(19) x

(20) 4* (3/4,0,0) x,-1/4,1/2  
(20) x

(21) 4* (0,3/4,0) 1/2,y,1/4  
(21) x

(22) 2 (3/4,0,3/4) x,1/8,x  
(22) x

(23) 4' (0,1/4,0) 0,y,1/4  
(23) x

(24) 2 (1/4,0,-1/4) x+1/2,3/8,x  
(24) x

(25) 1' 3/8,3/8,1/8  
(25) x

(26) d' (3/4,1/4,0) x,y,3/8  
(26) x

(27) d' (1/4,1/4,0) x,1/8,z  
(27) x

(28) d' (0,3/4,3/4) 1/8,y,z  
(28) x

(29) 3' x+1/2,x;  
(29) x

(30) 3' x-3/2,x+1,x;  
(30) x

(31) 3' x+1/2,x+1,x;  
(31) x

(32) 3' x+1/2,x,x;  
(32) x

(33) 3' x,x+1/2,x;  
(33) x

(34) 3' x+1/2,x-1/2,x;  
(34) x

(35) 3' x-1/2,x+1,x;  
(35) x

(36) 3' x+1,x;  
(36) x

(37) g' (-1/4,1/4,1/2) x+1/4,x,z  
(37) x

(38) g' (1/2,1/2,0) x,y,x  
(38) x

(39) 4' 1/4,1/4,z; 1/4,1/4,1/4  
(39) x

(40) g' 0,0,z; 0,0,0  
(40) x

(41) 4' x,0,1/2; 0,0,1/2  
(41) x

(42) m' x,y,y  
(42) x

(43) g' (1/2,1/4,1/4) x,y+1/4,y  
(43) x

(44) 4' x,1/4,1/4; 1/4,1/4,1/4  
(44) x

(45) 4' -1/4,y,1/4; -1/4,1/4,1/4  
(45) x

(46) m' x+1/2,y,x  
(46) x

(47) 4' 0,y,0; 0,0,0  
(47) x

(48) g' (1/4,1/2,1/4) x+1/4,y,x  
(48) x

Generators selected  
(1): t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

192 1

(1) x,y,z [u,v,w]  

(2) x,y+1/2,z+1/2 [u,v,w]  

(3) x+1/2,y+1/2,z [u,v,w]  

(4) x+1/2,y,z+1/2 [u,v,w]

(5) z,x,y [w,u,v]  

(6) z+1/2,x,y+1/2 [w,u,v]  

(7) z,x+1/2,y+1/2 [w,u,v]  

(8) z+1/2,x+1/2,y [w,u,v]

227.5.1632 - 4 - 3819
### Symmetry of Special Projections

| 8 | a | \(4\bar{3}m'\) | 0,0,0 | 3/4,1/4,3/4 [0,0,0] |
| 16 | d | \(\bar{3}m'\) | 5/8,5/8,5/8 [u,u,u] | 3/8,7/8,1/8 [u,u,u] | 7/8,1/8,3/8 [u,u,u] | 1/8,3/8,7/8 [u,u,u] |
| 16 | c | \(\bar{3}m'\) | 1/8,1/8,1/8 [u,u,u] | 7/8,3/8,5/8 [u,u,u] | 3/8,5/8,7/8 [u,u,u] | 5/8,7/8,3/8 [u,u,u] |

**Symmetry of Special Projections**

- **Along \([0,0,1]\)**
  - \(p4m'm'\)  
    - \(a^* = (a - b)/4\)  
    - \(b^* = (a + b)/4\)  
    - Origin at 0,0,z

- **Along \([1,1,1]\)**
  - \(p6m'm'\)  
    - \(a^* = (2a - b - c)/6\)  
    - \(b^* = (-a + 2b - c)/6\)  
    - Origin at x,x,x

- **Along \([1,1,0]\)**
  - \(c2m'm'\)  
    - \(a^* = (-a + b)/2\)  
    - \(b^* = c\)  
    - Origin at x,x,1/8
Origin at center (3), at 3/8,3/8,3/8 from 23

Asymmetric unit
-1/8 ≤ x ≤ 3/8;  -1/8 ≤ y ≤ 0;  -1/4 ≤ z ≤ 0;  y ≤ min(1/4-x,x);  -y-1/4 ≤ z ≤ y

Vertices
-1/8,-1/8,-1/8  3/8,-1/8,-1/8  1/4,0,0  0,0,0  1/4,0,-1/4  0,0,-1/4

Symmetry Operations
For (0,0,0) + set

1 0,0,0  1 (1) 1  
(1) 0,1/2,0  1/8,3/8,3/8

(2) 2 0,1/2,0  1/8,3/8,3/8
(2) 0,1/2,0  1/8,3/8,3/8

(2) 1/4,3/4,1/2  1/4,3/4,1/2
(2) 1/4,3/4,1/2  1/4,3/4,1/2

(3) 3 0,0,0  0,0,0  0,0,0
(3) 3 0,0,0  0,0,0  0,0,0

(3) x,y,z  1/2,1/2,1/2
(3) x,y,z  1/2,1/2,1/2

(3) x,y,z  3/4,1/2,1/2
(3) x,y,z  3/4,1/2,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2

(3) x,y,z  1/4,3/4,1/2
(3) x,y,z  1/4,3/4,1/2
Continued

(13) \(2 \ (1/2,1/2,0) \ x,x-1/4,0 \)  
(2) \(3 \ x,x+1/2,1/4 \)  
(14) \(4 \ (0,0,3/4) \ 1/8,-1/8,z \)  
(15) \(4 \ (0,0,1/4) \ -3/8,3/8,z \)  
(16) \(4 \ (0,1/4,1/4) \ 1/4,0,3/4 \)

(17) \(4 \ (3/4,0,0) \ x,1/8,-1/8 \)  
(18) \(2 \ (0,1/2,1/2) \ 0,y+1/4,y \)  
(19) \(2 \ 1/4,y+1/2,y \)  
(20) \(4 \ (1/4,0,0) \ x,-3/8,3/8 \)  
(4) \(1/4,0,3/4 \)

(21) \(4 \ (0,1/4,0) \ 3/8,y,-3/8 \)  
(4) \(3/4,1/4,0 \)  
(22) \(2 \ (1/2,0,1/2) \ x-1/4,0,x \)  
(23) \(4 \ (0,3/4,0) \ -1/8,y,1/8 \)  
(4) \(1/4,0,3/4 \)  
(24) \(2 \ 1/2,1/2,1/2 \)

(25) \(\bar{1} \ 0,0,0 \)  
(26) \(d \ (3/4,1/4,0) \ x,y,1/4 \)  
(27) \(d \ (1/4,0,3/4) \ x,1/4,z \)  
(28) \(d \ (0,3/4,1/4) \ 1/4,y,z \)  
(29) \(3^+ \ x,x;x; \)  
(30) \(\bar{3} \ x,x,x; \)  
(31) \(\bar{3} \ x,x,x; \)  
(32) \(3^+ \ x,x,x; \)  
(33) \(\bar{3} \ x,x,x; \)  
(34) \(\bar{3} \ x,x,x; \)  
(35) \(\bar{3} \ x,x,x; \)  
(36) \(3^+ \ x,x,x; \)  
(37) \(g \ (-1/4,1/4,1/2) \ x+1/2,x,z \)  
(38) \(n \ (1/2,1/2,1/2) \ x,x,z \)  
(39) \(g \ (3/4,3/4,0) \ 1/4,3/4) \)  
(40) \(4 \ (1/8,1/8,z) \ 1/8,1/8,3/8 \)  
(4) \(1/4,0,3/4 \)

(41) \(4 \ (3/4,3/8,3/8) \ 1/8,3/8,3/8 \)  
(4) \(1/4,3/4,0 \)  
(42) \(g \ (0,-1/4,1/4) \ x,y+1/2,y \)  
(43) \(n \ (1/2,1/2,1/2) \ x,y,y \)  
(44) \(4 \ (1/8,1/8,z) \ 1/8,1/8,3/8 \)  
(4) \(1/4,0,3/4 \)

(45) \(4 \ (1/4,0,1/4) \ x+1/2,y,x \)  
(46) \(g \ (1/4,0,1/4) \ 1/8,1/8,3/8 \)  
(47) \(4 \ (1/4,0,1/4) \ 1/8,1/8,3/8 \)  
(48) \(n \ (1/2,1/2,1/2) \ x,y,x \)  
(4) \(1/4,0,3/4 \)

For \(0,1/2,1/2\) + set
Generators selected \[(1); \ t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

**Positions**

Multiplicity, Wyckoff letter, Site Symmetry.

\[192 \ h \ 1\]

(1) \(x,y,z \ [u,v,w]\)
(2) \(x+1/4,y+3/4,z+1/2 \ [u,v,w]\)
(3) \(x+3/4,y+1/2,z+1/4 \ [u,v,w]\)
(4) \(z+3/4,x+1/4,z+1/4 \ [u,v,w]\)
(5) \(z+1/2,x+1/4,y+3/4 \ [w,u,v]\)

\[228.1.1633 - 4 - 3825\]
Continued

<table>
<thead>
<tr>
<th>48</th>
<th>d</th>
<th>4..</th>
<th>7/8,1/8,1/8 [u,0,0]</th>
<th>3/8,5/8,5/8 [u,0,0]</th>
<th>1/8,7/8,1/8 [0,u,0]</th>
<th>5/8,3/8,5/8 [0,u,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/8,1/8,7/8 [0,0,u]</td>
<td>5/8,5/8,3/8 [0,0,u]</td>
<td>7/8,1/8,7/8 [0,u,0]</td>
<td>3/8,5/8,3/8 [0,u,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5/8,3/8,7/8 [u,0,0]</td>
<td>1/8,7/8,3/8 [u,0,0]</td>
<td>7/8,3/8,1/8 [0,0,u]</td>
<td>3/8,7/8,5/8 [0,u,0]</td>
</tr>
<tr>
<td>32</td>
<td>c</td>
<td>.3.</td>
<td>0,0,0 [u,u,u]</td>
<td>1/4,3/4,1/2 [u,u,u]</td>
<td>3/4,1/2,1/4 [u,u,u]</td>
<td>1/2,1/4,3/4 [u,u,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,1/4,0 [u,u,u]</td>
<td>1/2,1/2,1/2 [u,u,u]</td>
<td>1/4,0,3/4 [u,u,u]</td>
<td>0,3/4,1/4 [u,u,u]</td>
</tr>
<tr>
<td>32</td>
<td>b</td>
<td>.32</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
<td>1/2,3/4,0 [0,0,0]</td>
<td>3/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,1/4,0 [0,0,0]</td>
<td>1/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>16</td>
<td>a</td>
<td>23.</td>
<td>1/8,1/8,1/8 [0,0,0]</td>
<td>7/8,3/8,7/8 [0,0,0]</td>
<td>7/8,7/8,7/8 [0,0,0]</td>
<td>1/8,5/8,1/8 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

<table>
<thead>
<tr>
<th>Origin at 1/8,3/8,z</th>
<th>Along [0,0,1] p4m'm'</th>
<th>a* = (a - b)/4, b* = (a + b)/4</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (2a - b - c)/6</td>
<td>Origin at x,x,x</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Origin at x-1/4,x+1/4,0</th>
<th>Along [1,1,0] p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/4, b* = c/2</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Origin at x,x,x</th>
<th>Along [1,1,1] p6m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (2a - b - c)/6</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Origin at x,x,x</th>
<th>Along [1,1,0] p2mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>a* = (-a + b)/4, b* = c/2</td>
<td></td>
</tr>
</tbody>
</table>
Origin at center (31’), at 3/8,3/8,3/8 from 231’

Asymmetric unit
-1/8 ≤ x ≤ 3/8; -1/8 ≤ y ≤ 0; -1/4 ≤ z ≤ 0; y ≤ min(1/4-x,x); -y-1/4 ≤ z ≤ y

Vertices
-1/8,-1/8,-1/8 3/8,-1/8,-1/8 1/4,0,0 0,0,0 1/4,0,-1/4 0,0,-1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 0,0,0)

(5) 3' x,x,x
(3_{xyz} | 0,0,0)

(9) 3' x,x,x
(3_{xyz}^{-1} | 0,0,0)

(2) 2 (0,0,1/2) 1/8,3/8,z
(2_2 | 1/4,3/4,1/2)

(6) 3' (1/3,-1/3,1/3)
\bar{x}+1/6, \bar{x}+5/12, \bar{x}
(3_{xyz}^{-1} | 2,1/4,3/4)

(10) 3' x+1/4,x+1/2, \bar{x}
(3_{xyz} | 3/4,1/2,1/4)

(3) 2 (0,1/2,0) 3/8,y,1/8
(2_2 | 3/4,1/2,1/4)

(7) 3' (-1/3,1/3,1/3)
\bar{x}+7/12, \bar{x}-1/6, \bar{x}
(3_{xyz}^{-1} | 1/4,3/4,1/2)

(11) 3' \bar{x}+3/4, \bar{x}+1/4, x
(3_{xyz} | 1/2,1/4,3/4)

(4) 2 (1/2,0,0) x,1/8,3/8
(2_2 | 1/2,1/4,3/4)

(8) 3' (1/3,1/3,-1/3)
\bar{x}+5/12, \bar{x}+7/12, x
(3_{xyz}^{-1} | 3/4,1/2,1/4)

(12) 3' \bar{x}-1/2, x+3/4, \bar{x}
(3_{xyz}^{-1} | 1/4,3/4,1/2)
Continued 228.2.1634 Fd3c1'

(33) $\bar{3}$' x-1/2, x-1/2, x;
(34) $\bar{3}$' x+1/4, x-1/2, x;
(35) $\bar{3}$' x+1/4, x+5/4, x;
(36) $\bar{3}$' x+3/2, x-3/4, x;

(37) c (0, 0, 1/2) x+1/4, x, z
(m_{xy} | 1/4, 1/4, 1/2)

(38) g (1/4, 1/4, 0) x+1/4, x, z
(m_{xy} | 1/2, 0, 0)

(39) $\bar{4}$' 1/8, 5/8, z; 1/8, 5/8, 3/8
($ m_{yz} | 3, 1/4, 1/2$)

(40) $\bar{4}$' 3/8, 3/8, 3/8; 3/8, 3/8, 1/8
($ m_{yz} | 0, 3/4, 1/4$)

(41) $\bar{4}$' x, -1/8, 3/8; 1/8, -1/8, 3/8
($ m_{yz} | 0, 3/4, 1/4$)

(42) g (0, 1/4, -1/4) x, y+1/2, y
($ m_{yz} | 0, 3/4, 1/4$)

(43) a (1/2, 0, 0) x, y, y
($ m_{yz} | 1/2, 0, 0$)

(44) $\bar{4}$' x, 5/8, 1/8; 3/8, 5/8, 1/8
($ m_{yz} | 3, 0, 3/4$)

(45) $\bar{4}$' -1/8, y, 3/8; -1/8, 1/8, 3/8
($ m_{xy} | 3/4, 1/4, 1/2$)

(46) b (0, 1/2, 0) x+3/4, y, x
($ m_{xy} | 3/4, 1/2, 3/4$)

(47) $\bar{4}$' 1/8, y, 1/8; 1/8, 3/8, 1/8
($ m_{xy} | 0, 3/4, 1/4$)

(48) g (1/4, 0, 1/4) x+1/4, y, x
($ m_{xy} | 1/2, 0, 0$)

For (1/2, 0, 1/2) + set

(1) t (1/2, 0, 1/2)

(2) 2 3/8, 3/8, z

(3) 2 (0, 1/2, 0) 1/8, y, 3/8

(4) 2 x, 1/8, 1/8

(5) $3^+$ (1/3, 1/3, 1/3) x+1/6, x-1/6, x
($ m_{xy} | 1/2, 0, 1/2$)

(6) $3^+$ x, x+1/4, x

(7) $3^+$ x+3/4, x, x

(8) $3^+$ x+1/4, x+3/4, x

(9) 3 (1/3, 1/3, 1/3) x+1/6, x-1/3, x
($ m_{xy} \mid 1/2, 0, 1/2$)

(10) 3' (-1/3, 1/3, 1/3) x+5/12, x+1/6, x

(11) 3' x+1/4, x+1/4, x

(12) 3' x, x+3/4, x

(13) 2 (1/4, 1/4, 0) x, x, 1/4

(14) 2 (-1/4, 1/4, 0) x, x+1/4, 0

(15) 4' (0, 0, 1/4) 3/8, -3/8, z

(16) $4^*$ (0, 0, 3/4) -1/8, 5/8, z

(17) 4' (1/4, 0, 0) x, 3/8, 1/8

(18) 2 (0, 3/4, 3/4) 1/4, y, y

(19) 2 (0, 1/4, -1/4) 0, y+1/4, y

(20) 4' (3/4, 0, 0) x, -1/8, 1/8

(21) $4^*$ (0, 1/4, 0) 3/8, y, 1/8

(22) 2 (1/2, 0, 1/2) x+1/4, 0, x

(23) $4^*$ (0, 3/4, 0) -1/8, y, 5/8

(24) 2 x, 1/4, x

(25) $\bar{1}$ 1/4, 0, 1/4

(26) d (1/4, 1/4, 0) x, y, 0

(27) d (3/4, 0, 1/4) x, 1/4, z

(28) d (0, 3/4, 3/4) 0, y, z

(29) $\bar{3}$' x-1/2, x-1/2, x;

(30) $\bar{3}$' x-3/2, x+3/4, x;

(31) $\bar{3}$' x-1/4, x+1/2, x;

(32) $\bar{3}$' x+3/4, x-1/4, x;

(33) $\bar{3}$' x+1/2, x, x;

(34) $\bar{3}$' x+5/4, x-1, x;

(35) $\bar{3}$' x-3/4, x+3/4, x;

(36) $\bar{3}$' x+1/2, x-1/4, x;

(37) c (0, 0, 1/2) x+3/4, x, z

(38) g (1/4, 1/4, 0) x-1/4, x, z

(39) $\bar{4}'$ 1/8, 1/8, z; 1/8, 1/8, 3/8

(40) $\bar{4}'$ 3/8, -1/8, z; 3/8, 1/8, 1/8

(41) $\bar{4}'$ x, 1/8, 5/8; 3/8, 1/8, 5/8

(42) a (1/2, 0, 0) x, y+1/4, y

(43) g (0, 1/4, 1/4) x, y+1/4, y

(44) $\bar{4}'$ x, 3/8, 3/8; 1/8, 3/8, 3/8

(45) $\bar{4}'$ 1/8, y, 5/8; 1/8, 3/8, 5/8

(46) b (1/4, 0, 1/4) x+1/2, y, x

(47) $\bar{4}'$ 3/8, y, -1/8; 3/8, 1/8, -1/8

(48) b (0, 1/2, 0) x, y, x
Continued 228.2.1634 Fd\(^{3}\)c1'

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>192 h 11'</td>
<td>(0,0,0) + (0,1/2,1/2,) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td></td>
<td>(0,0,0)' + (0,1/2,1/2,')' + (1/2,0,1/2') + (1/2,1/2,0')' +</td>
</tr>
</tbody>
</table>

| (1) x,y,z [0,0,0]                           | (2) x+1/4,y+3/4,z+1/2 [0,0,0] |
|                                           | (3) x+3/4,y+1/2,z+1/4 [0,0,0] |
|                                           | (4) x+1/2,y+1/4,z+3/4 [0,0,0] |
| (5) z,x,y [0,0,0]                           | (6) z+1/2,x+1/4,y+3/4 [0,0,0] |
|                                           | (7) z+1/4,x+3/4,y+1/2 [0,0,0] |
|                                           | (8) z+3/4,x+1/2,y+1/4 [0,0,0] |
| (9) y,z,x [0,0,0]                           | (10) y+3/4,z+1/2,x+1/4 [0,0,0] |
|                                           | (11) y+1/2,z+1/4,x+3/4 [0,0,0] |
|                                           | (12) y+1/4,z+3/4,x+1/2 [0,0,0] |
| (13) y+3/4,x+1/4,z [0,0,0]                 | (14) y+1/2,x+1/2,z+1/2 [0,0,0] |
|                                           | (15) y+1/4,x,z+3/4 [0,0,0] |
|                                           | (16) y+3/4,z+1/4 [0,0,0] |
| (17) x+3/4,z+1/4,y [0,0,0]                 | (18) x,z+3/4,y+1/4 [0,0,0] |
|                                           | (19) x+1/2,z+1/2,y+1/2 [0,0,0] |
|                                           | (20) x+1/4,z,y+3/4 [0,0,0] |

228.2.1634 - 7 - 3834
<table>
<thead>
<tr>
<th>228.2.1634</th>
<th>Fd$^3$c1$'$</th>
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<tbody>
<tr>
<td>(21) $z+3/4,y+1/4,x$ [0,0,0]</td>
<td>(22) $z+1/4,y,x+3/4$ [0,0,0]</td>
</tr>
<tr>
<td>(25) $x,y,z$ [0,0,0]</td>
<td>(26) $x+3/4,y+1/4,z+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>(29) $\bar{z},x,y$ [0,0,0]</td>
<td>(30) $\bar{z}+1/2,x+3/4,y+1/4$ [0,0,0]</td>
</tr>
<tr>
<td>(33) $\bar{y},z,x$ [0,0,0]</td>
<td>(34) $y+1/4,z+1/2,x+3/4$ [0,0,0]</td>
</tr>
<tr>
<td>(37) $\bar{y}+1/4,x+3/4,z$ [0,0,0]</td>
<td>(38) $y+1/2,x+1/2,z+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>(41) $x+y+1/4,z+3/4,y$ [0,0,0]</td>
<td>(42) $x,z+1/4,y+3/4,x$ [0,0,0]</td>
</tr>
<tr>
<td>(45) $\bar{z}+1/4,y+3/4,x$ [0,0,0]</td>
<td>(46) $z+3/4,y,x+1/4$ [0,0,0]</td>
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<table>
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<tr>
<th>96</th>
<th>g</th>
<th>.21'</th>
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</thead>
<tbody>
<tr>
<td>1/4,y,$y$ [0,0,0]</td>
<td>$0,\bar{y}+3/4,y+1/2$ [0,0,0]</td>
<td>$1/2,y+1/2,y+1/4$ [0,0,0]</td>
</tr>
<tr>
<td>$\bar{y},1/4,y$ [0,0,0]</td>
<td>$\bar{y}+1/2,0,y+3/4$ [0,0,0]</td>
<td>$y+1/4,1/2,y+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$y,\bar{y},1/4$ [0,0,0]</td>
<td>$y+3/4,\bar{y}+1/2,0$ [0,0,0]</td>
<td>$y+1/2,\bar{y}+1/4,1/2$ [0,0,0]</td>
</tr>
<tr>
<td>3/4, $y,y$ [0,0,0]</td>
<td>$0,y+1/4,y+1/2$ [0,0,0]</td>
<td>$1/2,\bar{y}+1/2,\bar{y}+3/4$ [0,0,0]</td>
</tr>
<tr>
<td>$y,3/4,y$ [0,0,0]</td>
<td>$y+1/2,0,y+1/4$ [0,0,0]</td>
<td>$\bar{y}+3/4,1/2,\bar{y}+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$\bar{y},y,3/4$ [0,0,0]</td>
<td>$y+1/4,\bar{y}+1/2,0$ [0,0,0]</td>
<td>$\bar{y}+1/2,\bar{y}+3/4,1/2$ [0,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>96</th>
<th>f</th>
<th>2..1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,1/8,1/8 [0,0,0]</td>
<td>$x+1/4,5/8,5/8$ [0,0,0]</td>
<td>$1/8,x+1/8$ [0,0,0]</td>
</tr>
<tr>
<td>1/8,1/8,x [0,0,0]</td>
<td>$5/8,5/8,\bar{x}+1/4$ [0,0,0]</td>
<td>$7/8,\bar{x}+1/4,7/8$ [0,0,0]</td>
</tr>
<tr>
<td>x+3/4,3/8,7/8 [0,0,0]</td>
<td>$\bar{x},7/8,3/8$ [0,0,0]</td>
<td>$7/8,3/8,\bar{x}$ [0,0,0]</td>
</tr>
<tr>
<td>x,7/8,7/8 [0,0,0]</td>
<td>$x+3/4,3/8,3/8$ [0,0,0]</td>
<td>$7/8,\bar{x},7/8$ [0,0,0]</td>
</tr>
<tr>
<td>7/8,7/8,\bar{x} [0,0,0]</td>
<td>$3/8,3/8,x+3/4$ [0,0,0]</td>
<td>$1/8,\bar{x}+3/4,1/8$ [0,0,0]</td>
</tr>
<tr>
<td>$\bar{x}+1/4,5/8,1/8$ [0,0,0]</td>
<td>$x,1/8,5/8$ [0,0,0]</td>
<td>$1/8,5/8,x$ [0,0,0]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>64</th>
<th>e</th>
<th>.3.1'</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,x,x [0,0,0]</td>
<td>$\bar{x}+1/4,\bar{x}+3/4,x+1/2$ [0,0,0]</td>
<td>$\bar{x}+1/4,\bar{x}+3/4,x+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$\bar{x}+3/4,x+1/2,x+1/4$ [0,0,0]</td>
<td>$x+1/2,x+1/4,\bar{x}+3/4$ [0,0,0]</td>
<td>$x+1/2,x+1/4,\bar{x}+3/4$ [0,0,0]</td>
</tr>
<tr>
<td>$x+3/4,x+1/4,\bar{x}$ [0,0,0]</td>
<td>$\bar{x}+1/2,\bar{x}+1/2,\bar{x}+1/2$ [0,0,0]</td>
<td>$\bar{x}+1/2,\bar{x}+1/2,\bar{x}+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$x+1/4,\bar{x}+1/2,x+3/4$ [0,0,0]</td>
<td>$\bar{x}+1/2,x+3/4,x+1/4$ [0,0,0]</td>
<td>$\bar{x}+1/2,x+3/4,x+1/4$ [0,0,0]</td>
</tr>
<tr>
<td>$\bar{x}+1/4,\bar{x}+3/4,x$ [0,0,0]</td>
<td>$x+1/2,x+1/2,x+1/2$ [0,0,0]</td>
<td>$x+1/2,x+1/2,x+1/2$ [0,0,0]</td>
</tr>
<tr>
<td>$\bar{x}+3/4,x,x+1/4$ [0,0,0]</td>
<td>$x,\bar{x}+1/4,x+3/4$ [0,0,0]</td>
<td>$x,\bar{x}+1/4,x+3/4$ [0,0,0]</td>
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</table>

228.2.1634 - 8 - 3835
228.2.1634

Fd$\overline{3}$c1'

Continued

<table>
<thead>
<tr>
<th>48</th>
<th>d</th>
<th>0.41'</th>
<th>7/8,1/8,1/8 [0,0,0]</th>
<th>3/8,5/8,5/8 [0,0,0]</th>
<th>1/8,7/8,1/8 [0,0,0]</th>
<th>5/8,3/8,5/8 [0,0,0]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/8,1/8,7/8 [0,0,0]</td>
<td>5/8,5/8,3/8 [0,0,0]</td>
<td>7/8,1/8,7/8 [0,0,0]</td>
<td>3/8,5/8,3/8 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5/8,3/8,7/8 [0,0,0]</td>
<td>1/8,7/8,3/8 [0,0,0]</td>
<td>7/8,3/8,1/8 [0,0,0]</td>
<td>3/8,7/8,5/8 [0,0,0]</td>
</tr>
<tr>
<td>32</td>
<td>c</td>
<td>0.31'</td>
<td>0,0,0 [0,0,0]</td>
<td>1/4,3/4,1/2 [0,0,0]</td>
<td>3/4,1/2,1/4 [0,0,0]</td>
<td>1/2,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,1/4,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/4,0,3/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>32</td>
<td>b</td>
<td>0.321</td>
<td>1/4,1/4,1/4 [0,0,0]</td>
<td>0,1/2,3/4 [0,0,0]</td>
<td>1/2,3/4,0 [0,0,0]</td>
<td>3/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,3/4,3/4 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>1/2,1/4,0 [0,0,0]</td>
<td>1/4,0,1/2 [0,0,0]</td>
</tr>
<tr>
<td>16</td>
<td>a</td>
<td>23.1'</td>
<td>1/8,1/8,1/8 [0,0,0]</td>
<td>7/8,3/8,7/8 [0,0,0]</td>
<td>7/8,7/8,7/8 [0,0,0]</td>
<td>1/8,5/8,1/8 [0,0,0]</td>
</tr>
</tbody>
</table>

Symmetry of Special Projections

Along [0,0,1] p4mm1'

- $a^* = (a - b)/4$
- $b^* = (a + b)/4$
-Origin at 1/8,3/8,z

Along [1,1,1] p6mm1'

- $a^* = (2a - b - c)/6$
- $b^* = (-a + 2b - c)/6$
-Origin at x,x,x

Along [1,1,0] p2mm1'

- $a^* = (-a + b)/4$
- $b^* = c/2$
-Origin at x,x,0
Origin at center (3'), at 3/8,3/8,3/8 from 23

Asymmetric unit
-1/8 ≤ x ≤ 3/8; -1/8 ≤ y ≤ 0; -1/4 ≤ z ≤ 0; y ≤ min(1/4-x,x); -y-1/4 ≤ z ≤ y

Vertices
-1/8,-1/8,-1/8 3/8,-1/8,-1/8 1/4,0,0 0,0,0 1/4,0,-1/4 0,0,-1/4

Symmetry Operations
For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2 (0,0,1/2) 1/8,3/8,z (2) 1/4,3/4,1/2
(2) 1/4,3/4,1/2

(3) 2 (0,1/2,0) 3/8,y,1/8 (3) 3/4,1/2,1/4
(3) 3/4,1/2,1/4

(4) 2 (1/2,0,0) x,1/8,3/8 (4) 1/2,1/4,3/4
(4) 1/2,1/4,3/4

(5) 3' x,x,x
(5) 3',1/3,-1/3,1/3

X+1/6,x+5/12,x (3_1,1/2,1/4,3/4)
(3_1,1/2,1/4,3/4)

(6) 3' (1/3,-1/3,1/3) x+7/12,x-1/6,x (3_1^{-1},1/4,3/4,1/2)
(3_1^{-1},1/4,3/4,1/2)

(7) 3' (-1/3,1/3,1/3) (3_1^{-1},1/4,3/4,1/2)
(3_1^{-1},1/4,3/4,1/2)

(8) 3' (1/3,1/3,-1/3) x+5/12,x+7/12,x (3_1^{-1},3/4,1/2,1/4)
(3_1^{-1},3/4,1/2,1/4)

(9) 3' x,x,x
(9) 3',3/4,1/2,1/4

(3_1,3/4,1/2,1/4)
(3_1,3/4,1/2,1/4)

(10) 3' x+1/4,x+1/2,x (3_1,1/2,1/4,3/4)
(3_1,1/2,1/4,3/4)

(11) 3' x+3/4,x+1/4,x (3_1^{-1},1/4,3/4,1/2)
(3_1^{-1},1/4,3/4,1/2)

(12) 3' x-1/2,x+3/4,x (3_1^{-1},1/4,3/4,1/2)
(3_1^{-1},1/4,3/4,1/2)
Continued 228.3.1635 Fd$^3$3c

(33) $3' \cdot x-1/2, x-1/2, x$

(34) $3' \cdot x+1/4, x-1/2, x$

(35) $3' \cdot x+1/4, x+5/4, x$

(36) $3' \cdot x+3/2, x-3/4, x$

(37) $c(0,0,1/2) \quad x+1/4, x_\infty, z$

(38) $g(1/4,1/4,0) \quad x+1/4, x_\infty, z$

(39) $4' \cdot 1/8, 5/8, z; 1/8, 5/8, 3/8$

(40) $4' \cdot 3/8, 3/8, z; 3/8, 3/8, 1/8$

(41) $4' \cdot x-1/8, 3/8; 1/8, -1/8, 3/8$

(42) $g(0,1/4, -1/4) \quad x, y+1/2, y$

(43) $a(1/2,0,0) \quad x, y, y$

(44) $4' \cdot x, 5/8, 1/8; 3/8, 5/8, 1/8$

(45) $4' \cdot -1/8, y, 3/8; -1/8, 1/8, 3/8$

(46) $b(0,1/2,0) \quad x+3/4, y, x$

(47) $4' \cdot 1/8, y, 1/8; 1/8, 3/8, 1/8$

(48) $g(1/4,0,1/4) \quad x+1/4, y, x$

For $(1/2,0,1/2) + set$

(1) $t(1/2,0,1/2)$

(2) $2 \cdot 3/8, 3/8, z$

(3) $2 \cdot 0,1/2,0 \cdot 1/8, y, 3/8$

(4) $2 \cdot x, 1/8, 1/8$

(5) $3^+ (1/3,1/3,1/3)$

(6) $3^+ x, x+1/4, x$

(7) $3^+ x+3/4, x_\infty$

(8) $3^+ x+1/4, x_\infty+3/4, x$

(9) $3 \cdot (1/3,1/3,1/3)$

(10) $3' \cdot -1/3, 1/3, 1/3$

(11) $3' \cdot x+1/4, x+1/4, x$

(12) $3' \cdot x, x+3/4, x$

(13) $2' (1/4,1/4,0) \quad x, x, 1/4$

(14) $2' (-1/4,1/4,0) \quad x, x+1/4, 0$

(15) $4' \cdot (0,0,1/4) \quad 3/8, -3/8, z$

(16) $4' \cdot (0,0,3/4) \quad 1/4,0,3/4$}

(17) $4' (1/4,0,0) \quad x, 3/8, 1/8$

(18) $2' (0,3/4,3/4) \quad 1/4, y, y$

(19) $2' (0,1/4, -1/4) \quad 0, y+1/4, y$

(20) $4' \cdot (3/4,0,0) \quad x, -1/8, 1/8$

(21) $4' \cdot (0,1/4,0) \quad 3/8, y, 1/8$

(22) $2' (1/2,0,1/2) \quad x+1/4, 0, x$

(23) $4' \cdot (0,3/4,0) \quad -1/8, y, 5/8$

(24) $2' \cdot x, 1/4, x$

(25) $\tilde{1} \cdot 1/4, 0, 1/4$

(26) $d' (1/4,1/4,0) \quad x, y, 0$

(27) $d' (3/4,0,1/4) \quad x, 1/4, z$

(28) $d' (0,3/4,3/4) \quad 0, y, z$

(29) $3' \cdot x-1/2, x-1/2, x$

(30) $3' \cdot x-3/2, x+3/4, x$

(31) $3' \cdot x-1/4, x+1/2, x$

(32) $3' \cdot x+3/4, x-1/4, x$

(33) $3' \cdot x+1/2, x, x$

(34) $3' \cdot x+5/4, x, 1/4$

(35) $3' \cdot x+3/4, x+3/4, x$

(36) $3' \cdot x+1/2, x+1/4, x$

(37) $c(0,0,1/2) \quad x+3/4, \infty, z$

(38) $g(1/4,1/4,0) \quad x-1/4, x, z$

(39) $4' \cdot 1/8, 1/8, z; 1/8, 1/8, 3/8$

(40) $4' \cdot 3/8, -1/8, z; 3/8, -1/8, 1/8$

(41) $\overline{4} \cdot x, 1/8, 5/8; 3/8, 1/8, 5/8$

(42) $a(1/2,0,0) \quad x, y+1/4, y$

(43) $g(0,1/4,1/4) \quad x, y+1/4, y$

(44) $4' \cdot x, 3/8, 3/8; 1/8, 3/8, 3/8$

(45) $\overline{4} \cdot 1/8, y, 5/8; 1/8, 3/8, 5/8$

(46) $b(-1/4,0,1/4) \quad x+1/2, y, x$

(47) $\overline{4} \cdot 3/8, y, -1/8; 3/8, 1/8, -1/8$

(48) $b(0,1/2,0) \quad x, y, x$

(49) $(m_{xyz}) 1/4, 0, 1/2$
Continued 228.3.1635 Fd'3c

For (1/2,1/2,0) + set

<table>
<thead>
<tr>
<th>Positions</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t (1/2,1/2,0)</td>
<td>(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +</td>
</tr>
<tr>
<td>(1) 1/2,1/2,0</td>
<td></td>
</tr>
<tr>
<td>(5) 3* (1/3,1/3,1/3)</td>
<td>(3)* x+3/4,y+1/4,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(x+1/6,x+1/3,x)</td>
<td>(3)* x+3/4,y+1/4,z+1/2 [u,v,w]</td>
</tr>
<tr>
<td>(3)* x+3/4,y+1/4,z+1/2</td>
<td></td>
</tr>
<tr>
<td>(9) 3' (1/3,1/3,1/3)</td>
<td>(3') x+1/4,x+1/4,x+1/4</td>
</tr>
<tr>
<td>(x+1/3,x+1/6,x)</td>
<td>(3') x+1/4,x+1/4,x+1/4</td>
</tr>
<tr>
<td>(3)* x+1/4,x+1/4,x+1/4</td>
<td></td>
</tr>
</tbody>
</table>

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).
### Symmetry of Special Projections

**Along [0,0,1]**  
$p4'mm'$  
$a^* = (a - b)/4$  
$b^* = (a + b)/4$  
Origin at 1/8,3/8,z

**Along [1,1,1]**  
$p6mm$  
$a^* = (2a - b - c)/6$  
$b^* = (-a + 2b - c)/6$  
Origin at x,x,x

**Along [1,1,0]**  
$p2mm1'$  
$a^* = (-a + b)/4$  
$b^* = c/2$  
Origin at x,x,0

---

<table>
<thead>
<tr>
<th>48</th>
<th>d</th>
<th>4..</th>
<th>7/8,1/8,1/8 [u,0,0]</th>
<th>3/8,5/8,5/8 [u,0,0]</th>
<th>1/8,7/8,1/8 [0,u,0]</th>
<th>5/8,3/8,5/8 [0,0,u]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>1/8,1/8,7/8 [0,0,u]</td>
<td>5/8,5/8,3/8 [0,0,u]</td>
<td>7/8,1/8,7/8 [0,0,u]</td>
<td>3/8,5/8,3/8 [0,0,u]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5/8,3/8,7/8 [u,0,0]</td>
<td>1/8,7/8,3/8 [u,0,0]</td>
<td>7/8,3/8,1/8 [0,u,0]</td>
<td>3/8,7/8,5/8 [0,u,0]</td>
</tr>
<tr>
<td>32</td>
<td>c</td>
<td>.3'.</td>
<td>0,0,0 [0,0,0]</td>
<td>1/4,3/4,1/2 [0,0,0]</td>
<td>3/4,1/2,1/4 [0,0,0]</td>
<td>1/2,1/4,3/4 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,1/4,0 [0,0,0]</td>
<td>1/2,1/2,1/2 [0,0,0]</td>
<td>1/4,0,3/4 [0,0,0]</td>
<td>0,3/4,1/4 [0,0,0]</td>
</tr>
<tr>
<td>32</td>
<td>b</td>
<td>.32'</td>
<td>1/4,1/4,1/4 [u,u,u]</td>
<td>0,1/2,3/4 [u,u,u]</td>
<td>1/2,3/4,0 [u,u,u]</td>
<td>3/4,0,1/2 [u,u,u]</td>
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<td>3/4,3/4,3/4 [u,u,u]</td>
<td>0,1/2,1/4 [u,u,u]</td>
<td>1/2,1/4,0 [u,u,u]</td>
<td>1/4,0,1/2 [u,u,u]</td>
</tr>
<tr>
<td>16</td>
<td>a</td>
<td>23.</td>
<td>1/8,1/8,1/8 [0,0,0]</td>
<td>7/8,3/8,7/8 [0,0,0]</td>
<td>7/8,7/8,7/8 [0,0,0]</td>
<td>1/8,5/8,1/8 [0,0,0]</td>
</tr>
</tbody>
</table>
Origin at center (3), at 3/8,3/8,3/8 from 23

Asymmetric unit
-1/8 ≤ x ≤ 3/8;
-1/8 ≤ y ≤ 0;
-1/4 ≤ z ≤ 0;
y ≤ min(1/4-x,x);
-y-1/4 ≤ z ≤ y

Vertices
-1/8,-1/8,-1/8 3/8,-1/8,-1/8 1/4,0,0 0,0,0 1/4,0,-1/4 0,0,-1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1 | 0,0,0)

(5) 3+ x,x,x
(3_xyz | 0,0,0)

(9) 3+ x,x,x
(3_xyz⁻¹ | 0,0,0)

(2) 2 (0,0,1/2) 1/8,3/8,3/8 (2, 1/4,3/4,1/2)

(6) 3+ (1/3,-1/3,1/3)
\(x+1/6, x+5/12, x\) (3_xyz⁻¹ | 1/2, 1/4, 3/4)

(7) 3+ (-1/3,1/3,1/3)
\(x+7/12, x-1/6, x\) (3_xyz⁻¹ | 1/4, 3/4, 1/2)

(8) 3+ (1/3,1/3,-1/3)
\(x+5/12, x+7/12, x\) (3_xyz⁻¹ | 3/4, 1/2, 1/4)

(10) 3+ x+1/4, x+1/2, x (3_xyz | 3/4, 1/2, 1/4)

(11) 3+ x+3/4, x+1/4, x (3_xyz⁻¹ | 1/2, 1/4, 3/4)

(12) 3+ x+1/2, x+3/4, x (3_xyz⁻¹ | 1/4, 3/4, 1/2)
Continued

(13) $2^r (1/2, 1/2, 0, 0)$, $x, x+1/4, 0$

(14) $2^r (1/2, 1/2, 1/4)$, $x, x, x+1/2, 1/4$

(15) $4^s (0, 0, 3/4, 1/8, -1/8, 1/4, 0, 3/4, 3/4, 0)$

(16) $4^s (0, 1/4, 0, 0, 1/4, 3/4, 1/4, 0)$

(17) $4^s (3/4, 0, 0, 0)$, $x, 1/8, 1/8$

(18) $2^r (0, 1/2, 1/2, 0, 0, 1/4, y+1/4, y, x+1/2, 1/2, 1/4)$

(19) $2^r (1/2, 1/2, 1/4, 0, 1/4, 3/4, 0)$

(20) $4^s (1/4, 0, 0, 0, 1/4, 3/4, 1/4, 0)$

(21) $4^s (0, 1/4, 0, 0, 3/4, 1/4, 0)$, $x, 1/4, 0$

(22) $2^r (1/2, 0, 1/2, 0, 0, 1/4, 0, 1/4, 3/4, 4/4)$

(23) $4^s (0, 3/4, 0, 0, -1/8, 1/8, 1/4, 0, 1/4, 3/4, 1/4, 0)$

(24) $2^r (3/4, 1/4, 0, 0, 1/4, 3/4, 1/4, 0)$

(25) $1 \cdot 0, 0, 0$

(26) $d (3/4, 1/4, 0, 0, 1/4, 3/4, 1/4, 0)$

(27) $d (1/4, 0, 1/4, 0, 1/4, 3/4, 1/4, 0)$

(28) $d (0, 1/4, 1/4, 0, 1/4, 3/4, 1/4, 0)$

(29) $3^s 3, x, 0, 0$

(30) $3^s 3, x, x, 0, 0$

(31) $3^s 3, x, x, x, 0, 0$

(32) $3^s 3, x, x, x, 0, 0$

(33) $3^s 3, x, x, x, 0, 0$

(34) $3^s 3, x, x, x, 0, 0$

(35) $3^s 3, x, x, x, 0, 0$

(36) $3^s 3, x, x, x, 0, 0$

(37) $g' (1/4, 1/4, 1/4, 0, 0, 1/4, 3/4, 1/4, 0)$, $x, x, x, 0, 0, 1/4, 3/4, 1/4, 0$

(38) $n' (1/2, 1/2, 1/2, 0, 0, 1/4, 3/4, 1/4, 0)$, $x, x, x, 0, 0, 1/4, 3/4, 1/4, 0$

(39) $g' (1/4, 1/4, 1/4, 0, 0, 1/4, 3/4, 1/4, 0)$, $x, x, x, 0, 0, 1/4, 3/4, 1/4, 0$

(40) $g' (1/4, 1/4, 1/4, 0, 0, 1/4, 3/4, 1/4, 0)$, $x, x, x, 0, 0, 1/4, 3/4, 1/4, 0$

(41) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

(42) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

(43) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

(44) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

(45) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

(46) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

(47) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

(48) $4^s 4, 1/4, 3/4, 3/4, 0, 0, 1/4, 3/4, 1/4, 0$

For $(0, 1/2, 1/2, +)$ set
Continued

(1) t (1/2,1/2,0)
(1/2,1/2,0)

(2) 2 (0,0,1/2) 3/8,1/8,1/8
(2, 3/4,1/4,1/2)

(3) 2 1/8,1/8,1/8
(2, |1/4,0,1/4)

(4) 2 x,3/8,3/8
(2, |0,3/4,3/4)

(5) 3⁺ (1/3,1/3,1/3)

(6) 3⁺  x,x+3/4,x

(3, 0,3/4,3/4)

(7) 3⁺  x+3/4,x-1/2,x

(3, 1/4,1/4,1/2)

(8) 3⁺  x+1/4,x+1/4,x

(3, -1/4,0,1/4)

(9) 3' (1/3,1/3,1/3)

(10) 3'  x+1/4,x,x

(11) 3'  x+3/4,x+3/4,x

(12) 3' (1/3,-1/3,1/3)

(3, -1/6,x+7/12,x

(3, 1/4,1/4,1/2)

(13) 2' (1/2,1/2,0)

(14) 2'  x,x,1/4

(15) 4⁺  (0,0,3/4) 5/8,-1/8,z

(4, 3/4,1/2,3/4)

(16) 4⁺  (0,0,1/4) 1/8,3/8,z

(4, 1/2,1/4,1/4)

(17) 4⁺ (1/4,0,0)

(18) 2' (0,1/4,1/4)

(19) 2' (0,-1/4,1/4)

(20) 4⁺  (3/4,0,0)

(4, 3/4,1/2,3/4)

(21) 4⁺ (0,3/4,0)

(22) 2' (3/4,0,3/4)

(23) 4⁺  (1/4,0,0)

(4, 1/2,1/4,1/4)

(24) 2' (-1/4,0,1/4)

(2,0,0,1/2)

(25) 1/4,1/4,0

(26) d (1/4,3/4,0)

(27) d (3/4,0,3/4)

(28) d (0,1/4,1/4)

(29) 3⁺

(30) 3⁺  x+1/2,x,x;

(3, 1/2,0,0)

(3, -1/4,0,1/4)

(3, 0,3/4,3/4)

(3, 1/4,3/4,1/2)

(3, 0,1/4,1/4)

(3, 1/4,3/4,1/2)

(3) x+y,x+3/4,x; 0,1/2,0

(3, -1/4,0,1/4)

(3, 0,3/4,3/4)

(3, 1/4,3/4,1/2)

(3) x+1/2,x,z;

(3, 0,0,1/2)

(3, 0,1/2,1/2)

(3, 0,0,1/2)

(3, 0,1/2,1/2)

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

(3) x+y,x+3/4,x; 0,1/2,0

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(0,1/2,1/2); t(1/2,0,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

192 h 1

(1) x,y,z [u,v,w]

(2) x+1/4,y+3/4,z+1/2 [u,v,w]

(3) x+3/4,y+1/2,z+1/4 [u,v,w]

(4) x+1/2,y+1/4,z+3/4 [u,v,w]

(5) z,x,y [w,u,v]

(6) z+1/2,x+1/4,y+3/4 [w,u,v]

(7) z+1/4,x+3/4,y+1/2 [w,u,v]

(8) z+3/4,x+1/2,y+1/4 [w,u,v]
### Symmetry of Special Projections

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
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<th></th>
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</thead>
<tbody>
<tr>
<td>b</td>
<td>0,0,0</td>
<td>1/4,3/4,1/2</td>
<td>3/4,1/2,1/4</td>
<td>1/2,1/4,3/4</td>
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<tr>
<td>c</td>
<td>3/4,1/4,0</td>
<td>1/2,1/2,1/2</td>
<td>1/4,0,3/4</td>
<td>0,3/4,1/4</td>
</tr>
<tr>
<td>d</td>
<td>48</td>
<td>48</td>
<td>48</td>
<td>48</td>
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</tbody>
</table>

### Symmetry of Special Projections

<table>
<thead>
<tr>
<th>Along [0,0,1]</th>
<th>p4 4m'm'</th>
<th>Along [1,1,1]</th>
<th>p6mm'</th>
<th>Along [1,1,0]</th>
<th>p2m'm'</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a^* = (a - b)/4 )</td>
<td>( b^* = (a + b)/4 )</td>
<td>( a^* = (2a - b - c)/6 )</td>
<td>( b^* = (-a + 2b - c)/6 )</td>
<td>( a^* = (-a + b)/4 )</td>
<td>( b^* = c/2 )</td>
</tr>
</tbody>
</table>

Origin at 1/8,5/8,z | Origin at x,x,x | Origin at x,x,0
Origin at center (3’), at 3/8,3/8,3/8 from 23

Asymmetric unit
-1/8 ≤ x ≤ 3/8;
-1/8 ≤ y ≤ 0;
-1/4 ≤ z ≤ 0;
y ≤ min(1/4-x,x);
-y-1/4 ≤ z ≤ y

Vertices
-1/8,-1/8,-1/8
3/8,-1/8,-1/8
1/4,0,0
0,0,0
1/4,0,-1/4
0,0,-1/4

Symmetry Operations
For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2 (0,0,1/2) 1/8,3/8,z
(2) 1/4,3/4,1/2

(3) 2 (0,1/2,0) 3/8,y,1/8
(2) 3/4,1/2,1/4

(4) 2 (1/2,0,0) x,1/8,3/8
(2) 1/2,1/4,3/4

(5) 3’ x,x,x
(3) 1/3,-1/3,1/3

(6) 3’ (1/3,-1/3,1/3)
(3) 1/2,1/4,3/4

(7) 3’ (-1/3,1/3,1/3)
(3) 1/4,3/4,1/2

(8) 3’ (1/3,1/3,-1/3)
(3) 3/4,1/2,1/4

(9) 3’ x,x,x
(3) 0,0,0

(10) 3’ x+1/4,x+1/2,x
(3) 3/4,1/2,1/4

(11) 3’ x+3/4,x+1/4,x
(3) 1/2,1/4,3/4

(12) 3’ x-1/2,x+3/4,x
(3) 1/4,3/4,1/2
Continued 228.5.1637 Fd'3c'

| (33) | $\bar{3}$' x-1/2,x-1/2,x; |
| (34) | $\bar{3}$' x+1/4,x-1/2,x; |
| (35) | $\bar{3}$' x+1/4,x+5/4,x; |
| (36) | $\bar{3}$' x+3/2,x-3/4,x; |

| (37) | c' (0,0,1/2) x+1/4,x,z |
| (38) | g' (1/4,1/4,0) x+1/4,x,z |
| (39) | $\bar{4}$' 1/8,5/8,z; 1/8,5/8,3/8 |
| (40) | $\bar{4}$' 3/8,3/8,3/8; 3/8,3/8,1/8 |

| (41) | $\bar{4}$' x,-1/8,3/8; 1/8,-1/8,3/8 |
| (42) | g' (0,1/4,-1/4) x,y+1/2,y |
| (43) | a' (1/2,0,0) x,y,y |
| (44) | $\bar{4}$' x,5/8,1/8; 3/8,5/8,1/8 |

| (45) | $\bar{4}$' -1/8,y,3/8; -1/8,1/8,3/8 |
| (46) | b' (0,1/2,0) x+3/4,y,x |
| (47) | $\bar{4}$' 1/8,y,1/8; 1/8,3/8,1/8 |
| (48) | g' (1/4,0,1/4) x+1/4,y,x |

For (1/2,0,1/2) + set

| (1) | t (1/2,0,1/2) |
| (2) | 2 3/8,3/8,z |
| (3) | 0 (0,1/2,0) 1/8,y,3/8 |
| (4) | 2 x,1/8,1/8 |

| (5) | $3^*$ (1/3,1/3,1/3) |
| (6) | 3* $\bar{x},x+1/4,x$ |
| (7) | 3* x+3/4,$\bar{x},\bar{x}$ |
| (8) | 3* $\bar{x}+1/4,\bar{x}+3/4,x$ |

| (9) | $3$ (1/3,1/3,1/3) |
| (10) | 3* (-1/3,1/3,1/3) |
| (11) | 3* $\bar{x}+1/4,\bar{x}+3/4,x$ |
| (12) | 3* $\bar{x},x+3/4,\bar{x}$ |

| (13) | 2 (1/4,1/4,0) x,x,1/4 |
| (14) | 2 (-1/4,1/4,0) x,x+1/4,0 |
| (15) | 4* (0,0,1/4) 3/8,-3/8,z |
| (16) | 4* (0,0,3/4) -1/8,5/8,z |

| (17) | 4* (1/4,0,0) x,3/8,1/8 |
| (18) | 2 (0,3/4,3/4) 1/4,y,y |
| (19) | 2 (0,1/4,-1/4) 0,y+1/4,\bar{y} |
| (20) | 4* (3/4,0,0) x,-1/8,1/8 |

| (21) | 4* (0,1/4,0) 3/8,y,1/8 |
| (22) | 2 (1/2,0,1/2) x+1/4,0,x |
| (23) | 4* (0,3/4,0) -1/8,y,5/8 |
| (24) | 2 $\bar{x},1/4,x$ |

| (25) | $\bar{1}$ 1/4,0,1/4 |
| (26) | d' (1/4,1/4,0) x,y,0 |
| (27) | d' (3/4,0,1/4) x,1/4,z |
| (28) | d' (0,3/4,3/4) 0,y,z |

| (29) | $\bar{3}$' x-1/2,x-1/2,x; |
| (30) | $\bar{3}$' x+3/4,x+3/4,x; |
| (31) | $\bar{3}$' x-1/4,x+1/2,x; |
| (32) | $\bar{3}$' x+3/4,x-1/4,x; |

| (33) | $\bar{3}$' x+1/2,x,x; |
| (34) | $\bar{3}$' x+5/4,x+1/4,x; |
| (35) | $\bar{3}$' x-3/4,x+3/4,x; |
| (36) | $\bar{3}$' x+1/2,x-1/4,x; |

| (37) | c' (0,0,1/2) x+3/4,x,z |
| (38) | g' (1/4,1/4,0) x-1/4,x,z |
| (39) | $\bar{4}$' 1/8,8/18,z; 1/8,1/8,3/8 |
| (40) | $\bar{4}$' 3/8,-1/8,z; 3/8,-1/8,1/8 |

| (41) | $\bar{4}$' x,1/8,5/8; 3/8,1/8,5/8 |
| (42) | a' (1/2,0,0) x,y+1/4,y |
| (43) | g' (0,1/4,1/4) x,y+1/4,y |
| (44) | $\bar{4}$' x,3/8,3/8; 1/8,3/8,1/8 |

| (45) | $\bar{4}$' 1/8,y,5/8; 1/8,3/8,5/8 |
| (46) | g' (-1/4,0,1/4) x+1/2,y,x |
| (47) | $\bar{4}$' 3/8,y,-1/8; 3/8,1/8,1/8 |
| (48) | b' (0,1/2,0) x,y,x |

For (1/2,0,1/2) + set
Generators selected

For (1/2,1/2,0) + set

(1) t (1/2,1/2,0)
(2) 2 (0,0,1/2) 3/8,1/8,1/8
(3) 2 1/8,y,1/8
(4) 2 x,3/8,3/8
(1/2,1/2,0)
(3/4,1/4,1/2) 0,1/4,0,1/4
(0,3/4,3/4)

(5) 3' (1/3,1/3,1/3)
(6) 3' x,x+3/4,x
(7) 3' x+3/4,x-1/2,x
(8) 3' x+1/4,x+1/4,x
(3xz) 1/2,1/2,0)
(0,3/4,3/4)
(3/4,1/4,1/2) 1/4,0,1/4
(3xy)

(9) 3' (1/3,1/3,1/3)
(10) 3' x+1/4,x,x
(11) 3' x+3/4,x+3/4,x
(12) 3' (1/3,-1/3,1/3)
(3xz)-1 1/2,1/2,0)
(3/4,1/4,1/2)
(3xz)

(13) 2 (1/2,1/2,0) x,x+1/4,0
(2xy) 1/4,3/4,0
(14) 2 x,x+1/4,0
(2xy) 0,0,1/2
(15) 4' (0,0,3/4) 5/8,1/8,1/8
(4z) 3/4,1/2,3/4
(16) 4' (0,0,1/4) 1/8,3/8,z
(4z) 1/2,1/4,1/4

(17) 4' (1/4,0,0) x,3/8,-3/8
(4x) -1 1/4,3/4,0
(18) 2 (0,1/4,1/4) 1/4,y,y
(2xy) 1/2,1/4,1/4
(19) 2 (0,-1/4,1/4) 0,y+1/4,y
(2xy) 0,0,1/2
(20) 4' (3/4,0,0) x,-1/8,5/8
(4z) 3/4,1/2,3/4

(21) 4' (0,3/4,0) 1/8,y,-1/8
(4y) 1/4,3/4,0
(22) 2 (3/4,0,3/4) x,1/4,x
(2xy) 3/4,1/2,3/4
(23) 4' (0,1/4,0) 1/8,y,3/8
(4y) 1/2,1/4,1/4
(24) 2 (-1/4,0,1/4) x+1/4,0,x
(2xy) 0,0,1/2

(25) 1' 1/4,1/4,0
(1/2,1/2,0)
(26) d' (1/4,3/4,0) x,y,1/4
(2m) 1/4,3/4,1/2)
(27) d' (3/4,0,3/4) x,0,z
(2m) 3/4,0,3/4)
(28) d' (0,1/4,1/4) 0,y,z
(2m) 0,1/4,1/4)

(29) 3' x+1/2,x,x;
(30) 3' x+1/2,x+1/4,x;
(3yz) 1/2,1/2,0)
(31) 3' x+1/4,x+1,x;
(3yz) 0,1/4,1/4)
(32) 3' x+3/4,x-3/4,x;
(3yz) 3/4,-3/4,0
(3yz)

(33) 3' x,x+1/2,x;
(34) 3' x+3/4,x-3/2,x;
(3yz) 1/2,1/2,0)
(35) 3' x+1/4,x+1/4,x;
(3yz) 0,1/4,1/4)
(36) 3' x+1/4,x+1/4,x;
(3yz) 3/4,1/2,1/4
(3yz)

(37) g' (1/4,-1/4,0) x+1/2,x,x;
(38) c' (0,0,1/2) x,x,z
(myz) 3/4,1/4,0)
(39) 4' -1/8,3/8,z; -1/8,3/8,1/8
(4z) 1/4,1/2,1/4)
(40) 4' 5/8,1/8,z; 5/8,1/8,3/8
(4z) 1/2,3/4,3/4)

(41) 4' x,1/8,1/8; 3/8,1/8,1/8
(4y) 1/4,1/4,0)
(42) a' (1/2,0,0) x,y+3/4,y
(myz) 1/4,3/4,3/4)
(43) g' (0,1/4,1/4) x,y+1/4,y
(4y) 0,0,1/2)
(44) 4' x,3/8,-1/8; 1/8,3/8,-1/8
(4y) 1/4,1/2,1/4)

(45) 4' 3/8,3/8; 3/8,1/8,3/8
(4y) 3/4,1/4,0)
(46) b' (0,1/2,0) x+1/4,y,x
(myz) 1/4,1/2,1/4)
(47) 4' 5/8,y,1/8; 5/8,3/8,1/8
(4y) 1/2,3/4,3/4)
(48) g' (1/4,0,1/4) x-1/4,y,x
(myz) 0,0,1/2)

Positions

Multiplicity, Wyckoff letter, Site Symmetry.
192 h 1

(1) x,y,z [u,v,w]
(2) x+1/4,y+3/4,z+1/2 [u,v,w]
(3) x+3/4,y+1/2,z+1/2 [u,v,w]
(4) x+1/2,y+1/4,z+3/4 [u,v,w]
(5) z,y,x [w,u,v]
(6) z+1/2,x+1/4,y+3/4 [w,u,v]
(7) z+1/4,x+3/4,y+1/2 [w,u,v]
(8) z+3/4,x+1/2,y+1/4 [w,u,v]

228.5.1637 - 4 - 3852
Continued
228.5.1637

Fd'3 'c'

(9) y,z,x [v,w,u]  (10) y+3/4,z+1/2, x+1/4 [v,w,u] (11) y+1/2, z+1/4, x+3/4 [v,w,u] (12) y+1/4, z+3/4, x+1/2 [v,w,u]

(13) y+3/4,x+1/4, z [v,u,w]  (14) y+1/2, x+1/2, z+1/2 [v,u,w] (15) y+1/4, x, z+3/4 [v,u,w]  (16) y,x+3/4, z+1/4 [v,u,w]

(17) x+3/4,z+1/4, y [u,w,v]  (18) x, z+3/4, y+1/4 [u,w,v]  (19) x+1/2, z+1/2, y+1/2 [u,w,v]  (20) x+1/4, z, y+3/4 [u,w,v]

(21) z+3/4, y+1/4, x [w,v,u]  (22) z+1/4, y+1/4 [w,v,u]  (23) z, y+3/4, x+1/4 [w,v,u]  (24) z+1/2, y+1/2, x+1/2 [w,v,u]

(25) x, y, z [u,v,w]  (26) x+3/4, y+1/4, z+1/2 [u,v,w] (27) x+1/4, y+1/2, z+3/4 [u,v,w]  (28) x+1/2, y+3/4, z+1/4 [u,v,w]

(29) z, x, y [w,u,v]  (30) z+1/2, x+3/4, y+1/4 [w,u,v] (31) z+3/4, x+1/4, y+1/2 [w,u,v]  (32) z+1/4, x+1/2, y+3/4 [w,u,v]

(33) y, z, x [v,w,u]  (34) y+1/4, z+1/2, x+3/4 [v,w,u] (35) y+1/2, z+3/4, x+1/4 [v,w,u]  (36) y+3/4, z+1/4, x+1/2 [v,w,u]

(37) y+1/4, x+3/4, z [v,u,w]  (38) y+1/2, x+1/2, z+1/2 [v,u,w] (39) y+3/4, x, z+1/4 [v,u,w]  (40) y, x+1/4, z+3/4 [v,u,w]

(41) x+1/4, z+3/4, y [u,w,v]  (42) x, z+1/4, y+3/4 [u,w,v]  (43) x+1/2, z+1/2, y+1/2 [u,w,v]  (44) x+3/4, z, y+1/4 [u,w,v]

(45) z+1/4, y+3/4, x [w,v,u]  (46) z+3/4, y, x+1/4 [w,v,u] (47) z, y+1/4, x+3/4 [w,v,u]  (48) z+1/2, y+1/2, x+1/2 [w,v,u]

96  g  2...

1/4,y, y [0,v,v]  0, y+3/4, y+1/2 [0,v,v]  1/2, y+1/2, y+1/4 [0,v,v]  3/4, y+1/4, y+3/4 [0,v,v]

y, 1/4, y [v,0,v]  y+1/2, 0, y+3/4 [v,0,v]  y+1/4, 1/2, y+1/2 [v,0,v]  y+3/4, 3/4, y+1/4 [v,0,v]

y, y, 1/4 [v,v,0]  y+3/4, y+1/2, 0 [v,v,0]  y+1/2, y+1/4, 1/2 [v,v,0]  y+1/4, y+3/4, 3/4 [v,v,0]

3/4, y, y [0,v,0]  0, y+1/4, y+1/2 [0,v,0]  1/2, y+1/2, y+3/4 [0,v,0]  1/4, y+3/4, y+1/4 [0,v,0]

y, 3/4, y [v,0,v]  y+1/2, 0, y+1/4 [v,0,v]  y+3/4, 1/2, y+1/2 [v,0,v]  y+1/4, 1/4, y+3/4 [v,0,v]

y, y, 3/4 [v,v,0]  y+1/4, y+1/2, 0 [v,v,0]  y+1/2, y+3/4, 1/2 [v,v,0]  y+3/4, y+1/4, 1/4 [v,v,0]

96  f  2...

x, 1/8, 1/8 [u,0,0]  x+1/4, 5/8, 5/8 [u,0,0]  1/8, x, 1/8 [0,u,0]  5/8, x+1/4, 5/8 [0,u,0]

1/8, 1/8, x [0,0,u]  5/8, 5/8, x+1/4 [0,0,u]  7/8, x+1/4, 7/8 [0,u,0]  3/8, x+1/2, 3/8 [0,u,0]

x, 3/4, 3/4, 7/8 [u,0,0]  x, 7/8, 3/8 [u,0,0]  7/8, 3/8, x [0,0,u]  3/8, 7/8, x+3/4 [0,0,u]

x, 7/8, 7/8 [u,0,0]  x+3/4, 3/4, 3/8 [u,0,0]  7/8, x, 7/8 [0,u,0]  3/8, x+3/4, 3/8 [0,u,0]

7/8, 7/8, x [0,0,u]  3/8, 3/8, x+3/4 [0,0,u]  1/8, x+3/4, 1/8 [0,u,0]  5/8, x+1/2, 5/8 [0,u,0]

x+1/4, 5/8, 1/8 [u,0,0]  x+1/4, 1/8, 5/8 [u,0,0]  1/8, 5/8, x [0,u,0]  5/8, 1/8, x+1/4 [0,u,0]

64  e  .3.

x, x, x [u,u,u]  x+1/4, x+3/4, x+1/2 [u,u,u]

x+3/4, x+1/2, x+1/4 [u,u,u]  x+1/2, x+1/4, x+3/4 [u,u,u]

x+3/4, x+1/4, x [u,u,u]  x+1/2, x+1/2, x+1/2 [u,u,u]

x+1/4, x, x+3/4 [u,u,u]  x, x+3/4, x+1/4 [u,u,u]

x, x, x [u,u,u]  x+3/4, x+1/4, x+1/2 [u,u,u]

x+1/4, x+1/2, x+3/4 [u,u,u]  x+1/2, x+3/4, x+1/4 [u,u,u]
Continued

\[ \begin{align*}
\bar{x} + 1/4, x + 3/4, x & \quad [u, u, u] \\
\bar{x} + 3/4, x + 1/4 & \quad [u, u, u] \\
\bar{x}, x + 1/4, x + 3/4 & \quad [u, u, u]
\end{align*} \]

48  d  \( \bar{4}' \cdot \)  
\[ \begin{align*}
7/8, 1/8, 1/8 & \quad [0, 0, 0] \\
1/8, 1/8, 7/8 & \quad [0, 0, 0] \\
5/8, 3/8, 7/8 & \quad [0, 0, 0]
\end{align*} \]

32  c  \( .3' \cdot \)  
\[ \begin{align*}
0, 0, 0 & \quad [0, 0, 0] \\
1/4, 3/4, 1/2 & \quad [0, 0, 0] \\
3/4, 1/4, 0 & \quad [0, 0, 0]
\end{align*} \]

32  b  \( .32 \)  
\[ \begin{align*}
1/4, 1/4, 1/4 & \quad [0, 0, 0] \\
3/4, 3/4, 3/4 & \quad [0, 0, 0]
\end{align*} \]

16  a  23.  
\[ \begin{align*}
1/8, 1/8, 1/8 & \quad [0, 0, 0] \\
1/8, 7/8, 1/8 & \quad [0, 0, 0]
\end{align*} \]

**Symmetry of Special Projections**

Along \([0,0,1]\)  p4m'm'  
\[ \begin{align*}
a^* &= (a - b)/4 \\
b^* &= (a + b)/4
\end{align*} \]
Origin at 1/8,3/8,z

Along \([1,1,1]\)  p6m'm'  
\[ \begin{align*}
a^* &= (2a - b - c)/6 \\
b^* &= (-a + 2b - c)/6
\end{align*} \]
Origin at x,x,x

Along \([1,1,0]\)  p2m'm'  
\[ \begin{align*}
a^* &= (-a + b)/4 \\
b^* &= c/2
\end{align*} \]
Origin at x,x,0
Origin at center (m\text{3}m)

Asymmetric unit

\[0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y \leq x; \quad z \leq \min(1/2-x,y)\]

Vertices

<table>
<thead>
<tr>
<th></th>
<th>0,0,0</th>
<th>1/2,0,0</th>
<th>1/2,1/2,0</th>
<th>1/4,1/4,1/4</th>
</tr>
</thead>
</table>

Symmetry Operations

For \((0,0,0) + \text{set}\)

1. \((1) \ 1\)
2. \((2) \ 0,0,z\)
3. \((2) \ 0,y,0\)
4. \((2) \ 0,0,0\)

5. \((3) \ x,x,x\)
6. \((3) \ x,x,x\)
7. \((3) \ x,x,x\)
8. \((3) \ x,x,x\)

9. \((3) \ x,x,x\)
10. \((3) \ x,x,x\)
11. \((3) \ x,x,x\)
12. \((3) \ x,x,x\)
<table>
<thead>
<tr>
<th>No.</th>
<th>Site Symmetry</th>
<th>Wyckoff letter, Site Symmetry</th>
<th>Generators selected</th>
</tr>
</thead>
<tbody>
<tr>
<td>33</td>
<td>3⁻ x,x,x; 1/4,1/4,1/4</td>
<td>(m_xz) 1/2,1/2,1/2</td>
<td>(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).</td>
</tr>
<tr>
<td>34</td>
<td>3⁻ x⁺1,x⁻1,x; 1/4,-1/4,3/4</td>
<td>(m_xz) 1/2,1/2,1/2</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>3⁻ x,x⁺1,x; -1/4,3/4,1/4</td>
<td>(m_xz) 1/2,1/2,1/2</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>3⁻ x⁺1,x,x; 3/4,1/4,-1/4</td>
<td>(m_xz) 1/2,1/2,1/2</td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>c (0,0,1/2) x⁺1/2,x,z</td>
<td>(m_yz) 1/2,1/2,1/2</td>
<td></td>
</tr>
<tr>
<td>38</td>
<td>n (1/2,1/2,1/2) x,x,z</td>
<td>(m_y) 1/2,1/2,1/2</td>
<td></td>
</tr>
<tr>
<td>39</td>
<td>4⁻ 0,1/2,z; 0,1/2,1/4</td>
<td>(m_y) 1/2,1/2,1/2</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>4⁺ 1/2,0,z; 1/2,0,1/4</td>
<td>(m_y) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>41</td>
<td>4⁻ x,0,1/2; 1/4,0,1/2</td>
<td>(m_yz) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>42</td>
<td>a (1/2,0,0) x⁺1/2,y,z</td>
<td>(m_y) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>43</td>
<td>n (1/2,1/2,1/2) x,y,y</td>
<td>(m_y) 1/2,1/2,1/2</td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>4⁺ x,1/2,0; 1/4,1/2,0</td>
<td>(m_y) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>45</td>
<td>4⁺ 0,y,1/2; 0,1/4,1/2</td>
<td>(m_yz) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>46</td>
<td>b (0,1/2,0) x⁺1/2,y,x</td>
<td>(m_y) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>47</td>
<td>4⁻ 1/2,y,0; 1/2,1/4,0</td>
<td>(m_y) 1/2,1/2,1/2</td>
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</tr>
<tr>
<td>48</td>
<td>n (1/2,1/2,1/2) x,y,x</td>
<td>(m_y) 1/2,1/2,1/2</td>
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</tbody>
</table>

Generators selected: (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.
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<tr>
<th>48</th>
<th>j</th>
<th>m..</th>
<th>0,y,z [u,0,0]</th>
<th>0,y,z [u,0,0]</th>
<th>0,y,z [u,0,0]</th>
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<td>y,z,0 [0,u,0]</td>
<td>y,z,0 [0,u,0]</td>
<td>y,z,0 [0,u,0]</td>
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<td>y,0,z [0,u,0]</td>
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<td>y,0,z [0,u,0]</td>
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<td>0,z,y [u,0,0]</td>
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<table>
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<tr>
<th>48</th>
<th>i</th>
<th>..2</th>
<th>1/4,y,y+1/2 [0,v,v]</th>
<th>3/4,y,y+1/2 [0,v,v]</th>
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</table>

<table>
<thead>
<tr>
<th>16</th>
<th>f</th>
<th>.3m</th>
<th>x,x,x [0,0,0]</th>
<th>x,x,x [0,0,0]</th>
<th>x,x,x [0,0,0]</th>
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<tr>
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<td>x,x,x [0,0,0]</td>
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<table>
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<tr>
<th>12</th>
<th>e</th>
<th>4m.m</th>
<th>x,0,0 [0,0,0]</th>
<th>x,0,0 [0,0,0]</th>
<th>x,0,0 [0,0,0]</th>
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<th>1/4,0,1/2 [0,0,0]</th>
<th>3/4,0,1/2 [0,0,0]</th>
<th>3/4,0,1/2 [0,0,0]</th>
<th>1/2,1/4,0 [0,0,0]</th>
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<td></td>
<td></td>
<td>1/2,3/4,0 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
<td>0,1/2,1/4 [0,0,0]</td>
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<tr>
<th>8</th>
<th>c</th>
<th>.3m</th>
<th>1/4,1,4/1 [0,0,0]</th>
<th>3/4,3/4,1/4 [0,0,0]</th>
<th>3/4,1/4,3/4 [0,0,0]</th>
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</thead>
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| 6  | b | 4/mm.m | 0,1/2,1/2 [0,0,0] | 1/2,0,1/2 [0,0,0] | 1/2,1/2,0 [0,0,0] | 1/2,1/2,0 [0,0,0] |

| 2  | a | m3m | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] | 0,0,0 [0,0,0] |
Symmetry of Special Projections

Along [0,0,1]  p4mm1'  
\[ a^* = \frac{(a - b)}{2}, \quad b^* = \frac{(a + b)}{2} \]
Origin at 0,0,z

Along [1,1,1]  p6'm'm  
\[ a^* = \frac{(2a - b - c)}{3}, \quad b^* = \frac{(-a + 2b - c)}{3} \]
Origin at x,x,x

Along [1,1,0]  p2mm1'  
\[ a^* = \frac{(-a + b)}{2}, \quad b^* = \frac{c}{2} \]
Origin at x,x,0
Im\textsuperscript{3}m1' \quad m\textsuperscript{3}m1' \quad \text{Cubic} \\
229.2.1639 \quad 14/m\textsuperscript{3}2/m1' \\

**Origin** at center (m\textsuperscript{3}m1')

**Asymmetric unit**

\begin{align*}
0 \leq x \leq 1/2; \\
0 \leq y \leq 1/2; \\
0 \leq z \leq 1/4; \\
y \leq x; \\
z \leq \min(1/2-x,y)
\end{align*}

**Vertices**

\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 1/4,1/4,1/4
\end{align*}

**Symmetry Operations**

For \((0,0,0) +\text{ set}\)

\begin{align*}
(1) & \quad 1 \\
(1) & \quad (1,0,0,0) \\
(5) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}[0,0,0]) \\
(9) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}^{-1}[0,0,0]) \\
(2) & \quad 2 \quad 0,0,z \\
& \quad (2,0,0,0) \\
(6) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}^{-1}[0,0,0]) \\
(10) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}[0,0,0]) \\
(3) & \quad 2 \quad 0,y,0 \\
& \quad (2,0,0,0) \\
(7) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}^{-1}[0,0,0]) \\
(11) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}[0,0,0]) \\
(4) & \quad 2 \quad x,0,0 \\
& \quad (2,0,0,0) \\
(8) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}^{-1}[0,0,0]) \\
(12) & \quad 3^+ x,x,x \\
& \quad (3_{xyz}[0,0,0])
\end{align*}
| 13 | $x, x, 0$ | 14 | $x, x, 0$ | 15 | $4^\ast, 0, 0, \bar{z}$ | 16 | $4^\ast, 0, 0, z$ |
| 17 | $4^\ast, x, 0, 0$ | 18 | $0, y, y$ | 19 | $2, 0, y, \bar{y}$ | 20 | $4^\ast, x, 0, 0$ |
| 21 | $4^\ast, 0, y, 0$ | 22 | $2, x, 0, x$ | 23 | $4^\ast, 0, y, 0$ | 24 | $2, \bar{x}, 0, x$ |
| 25 | $1, 0, 0, 0$ | 26 | $m, x, y, 0$ | 27 | $m, x, 0, z$ | 28 | $m, 0, y, z$ |
| 29 | $3^\ast, x, x, x; 0, 0, 0$ | 30 | $3^\ast, x, x, x; 0, 0, 0$ | 31 | $3^\ast, x, x, x; 0, 0, 0$ | 32 | $3^\ast, x, x, x; 0, 0, 0$ |
| 33 | $3^\ast, x, x, x; 0, 0, 0$ | 34 | $3^\ast, x, x, x; 0, 0, 0$ | 35 | $3^\ast, x, x, x; 0, 0, 0$ | 36 | $3^\ast, x, x, x; 0, 0, 0$ |
| 37 | $m, x, x, x$ | 38 | $m, x, x, x$ | 39 | $4^\ast, 0, 0, z; 0, 0, 0$ | 40 | $4^\ast, 0, 0, z; 0, 0, 0$ |
| 41 | $4^\ast, x, 0, 0; 0, 0, 0$ | 42 | $m, y, y, y$ | 43 | $m, x, y, y$ | 44 | $4^\ast, x, 0, 0; 0, 0, 0$ |
| 45 | $4^\ast, 0, y, 0; 0, 0, 0$ | 46 | $m, x, y, x$ | 47 | $4^\ast, 0, y, 0; 0, 0, 0$ | 48 | $m, x, y, x$ |

For $(1/2, 1/2, 1/2)$ + set

| 1 | $(1/2, 1/2, 1/2)$ | 2 | $(0, 0, 1/2)$ | 3 | $(0, 1/2, 0)$ | 4 | $(1/2, 0, 0)$ |
| 5 | $(1/2, 1/2, 1/2)$ | 6 | $(1, 6, -1, 6, 1, 6)$ | 7 | $3^\ast, (-1, 6, 1, 6, -1, 6)$ | 8 | $(1, 6, -1, 6, -1, 6)$ |
| 9 | $(1/2, 1/2, 1/2)$ | 10 | $(0, 1/2, 0)$ | 11 | $(1, 6, -1, 6, 1, 6)$ | 12 | $(1, 6, -1, 6, -1, 6)$ |
| 13 | $(1/2, 1/2, 2/2)$ | 14 | $(0, 1/2, 1/2)$ | 15 | $(0, 0, 1/2)$ | 16 | $(0, 0, 1/2)$ |
| 17 | $(1/2, 1/2, 0)$ | 18 | $(0, 1/2, 1/2)$ | 19 | $(0, 1/2, 1/2)$ | 20 | $(0, 1/2, 1/2)$ |
| 21 | $(1/2, 1/2, 1/2)$ | 22 | $(1, 6, 1, 6, -1, 6)$ | 23 | $(1, 6, -1, 6, 1, 6)$ | 24 | $(1, 6, -1, 6, -1, 6)$ |
| 25 | $(1/2, 1/2, 2/2)$ | 26 | $(0, 1/2, 0)$ | 27 | $(0, 1/2, 0)$ | 28 | $(0, 1/2, 0)$ |
| 29 | $(3, 1/2, 1/2, 2/2)$ | 30 | $(3, 1/2, 1/2, 2/2)$ | 31 | $(3, 1/2, 1/2, 2/2)$ | 32 | $(3, 1/2, 1/2, 2/2)$ |
Continued

(5) \(3^+\) (1/2,1/2,1/2) x,x,x

(9) \(3^-\) (1/2,1/2,1/2) x,x,x

(13) 2' (1/2,1/2,2) x,x,1/4

(17) 4^- (0,1/2,0) x,1/2,0

(21) \(\bar{1}\) 1/4,1/4,1/4

(25) \(\bar{3}\) x,x,x;

(29) \(\bar{3}^+\) x,x,x;

(33) \(\bar{3}^-\) x,x,x;

(37) \(c'\) (0,0,1/2) x+1/2,x,z

(41) \(\bar{4}\) x,0,1/2; 1/4,0,1/2

(45) \(\bar{4}^-\) 0,y,1/2; 0,1/4,1/2

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25); 1'.

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

Coordinates

\[ (0,0,0) + (1/2,1/2,1/2) + (0,0,0)' + (1/2,1/2,1/2)' + \]

\[ (1,0,0), (0,1,0), (0,0,1), t(1/2,1/2,1/2), (2), (3), (5), (13), (25), 1'. \]
(17) $x, z, y \ [0,0,0]$
(18) $ar{x}, z, y \ [0,0,0]$
(19) $x, z, \bar{y} \ [0,0,0]$
(20) $x, z, y \ [0,0,0]$

(21) $z, y, x \ [0,0,0]$
(22) $z, \bar{y}, x \ [0,0,0]$
(23) $\bar{z}, y, x \ [0,0,0]$
(24) $\bar{z}, \bar{y}, x \ [0,0,0]$

(25) $\bar{x}, \bar{y}, z \ [0,0,0]$
(26) $x, y, \bar{z} \ [0,0,0]$
(27) $x, \bar{y}, z \ [0,0,0]$
(28) $\bar{x}, y, z \ [0,0,0]$

(29) $\bar{z}, x, y \ [0,0,0]$
(30) $\bar{z}, x, \bar{y} \ [0,0,0]$
(31) $z, x, \bar{y} \ [0,0,0]$
(32) $z, x, y \ [0,0,0]$

(33) $y, z, x \ [0,0,0]$
(34) $y, z, x \ [0,0,0]$
(35) $\bar{y}, z, x \ [0,0,0]$
(36) $y, z, \bar{x} \ [0,0,0]$

(37) $\bar{y}, x, z \ [0,0,0]$
(38) $y, x, z \ [0,0,0]$
(39) $\bar{y}, x, \bar{z} \ [0,0,0]$
(40) $y, \bar{x}, z \ [0,0,0]$

(41) $\bar{x}, \bar{z}, y \ [0,0,0]$
(42) $x, \bar{z}, y \ [0,0,0]$
(43) $x, z, y \ [0,0,0]$
(44) $\bar{x}, z, \bar{y} \ [0,0,0]$

(45) $\bar{z}, y, x \ [0,0,0]$
(46) $\bar{z}, y, x \ [0,0,0]$
(47) $\bar{z}, y, x \ [0,0,0]$
(48) $\bar{z}, y, x \ [0,0,0]$

48 $k$ $m'1' \quad x, x, z \ [0,0,0]$
$\bar{x}, \bar{x}, z \ [0,0,0]$
$\bar{x}, \bar{z}, z \ [0,0,0]$
$x, z, \bar{x} \ [0,0,0]$

48 $j$ $m'1' \quad 0, y, z \ [0,0,0]$
$0, \bar{y}, z \ [0,0,0]$
$0, y, \bar{z} \ [0,0,0]$
$0, \bar{y}, \bar{z} \ [0,0,0]$

48 $i$ $..21'$
$\frac{1}{4}, y, \bar{y}+1/2 \ [0,0,0]$
$3/4, \bar{y}, \bar{y}+1/2 \ [0,0,0]$
$3/4, y, y+1/2 \ [0,0,0]$
$1/4, \bar{y}, y+1/2 \ [0,0,0]$

$y+1/2, 1/4, y \ [0,0,0]$
$\bar{y}+1/2, 3/4, \bar{y} \ [0,0,0]$
y+1/2, 3/4, y \ [0,0,0]$
$y+1/2, 1/4, \bar{y} \ [0,0,0]$

$\frac{3}{4}, \bar{y}+1/2 \ [0,0,0]$
$1/4, y, \bar{y}+1/2 \ [0,0,0]$
$1/4, \bar{y}, y+1/2 \ [0,0,0]$
$3/4, y, \bar{y}+1/2 \ [0,0,0]$

$y+1/2, 3/4, \bar{y} \ [0,0,0]$
$\bar{y}+1/2, 1/4, \bar{y} \ [0,0,0]$
$\bar{y}+1/2, 1/4, y \ [0,0,0]$
$\bar{y}+1/2, 3/4, y \ [0,0,0]$

$y+1/2, 3/4, y \ [0,0,0]$
$\bar{y}+1/2, 1/4 \ [0,0,0]$
$\bar{y}, \bar{y}+1/2, 1/4 \ [0,0,0]$
${y, \bar{y}+1/2, 3/4} \ [0,0,0]$
Symmetry of Special Projections

Along $[0,0,1]$ p4mm1'  
$a^* = (a - b)/2$  
$b^* = (a + b)/2$  
Origin at 0,0,z

Along $[1,1,1]$ p6mm1'  
$a^* = (2a - b - c)/3$  
$b^* = (-a + 2b - c)/3$  
Origin at x,x,x

Along $[1,1,0]$ p2mm1'  
$a^* = (-a + b)/2$  
$b^* = c/2$  
Origin at x,x,0
Origin at center (m'3'm)

Asymmetric unit

\[ 0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y \leq x; \quad z \leq \min(1/2-x,y) \]

Vertices

\[
\begin{align*}
0,0,0 & \quad 1/2,0,0 & \quad 1/2,1/2,0 & \quad 1/4,1/4,1/4
\end{align*}
\]

Symmetry Operations

For \((0,0,0) + \) set

\[
\begin{align*}
(1) & \quad 1 & \quad (2) & \quad 2 \ 0,0,z & \quad (3) & \quad 2 \ y,0,0 & \quad (4) & \quad 2 \ x,0,0 \\
& \quad (1) & \quad (2) & \quad (2) & \quad (2) & \quad (2) & \quad (2)
\end{align*}
\]

\[
\begin{align*}
(5) & \quad 3^+ \ x,x,x & \quad (6) & \quad 3^+ \ x,x,x & \quad (7) & \quad 3^+ \ x,x,x & \quad (8) & \quad 3^+ \ x,x,x \\
& \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz})
\end{align*}
\]

\[
\begin{align*}
(9) & \quad 3^- \ x,x,x & \quad (10) & \quad 3^- \ x,x,x & \quad (11) & \quad 3^- \ x,x,x & \quad (12) & \quad 3^- \ x,x,x \\
& \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz}) & \quad (3_{xyz})
\end{align*}
\]
Continued

Positions

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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
<tr>
<td>96</td>
<td>I</td>
<td>1</td>
</tr>
</tbody>
</table>

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

Generators selected

(1): t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

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<th>48</th>
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<th>m'</th>
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<th>229.3.1640</th>
<th>Im'3m</th>
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<tr>
<td>0, y, z [0, v, w]</td>
<td>3/4, y, y + 1/2 [u, v, v]</td>
<td>0, y, y [0, v, v]</td>
<td>0, y, y [0, v, v]</td>
<td>0, y, z [0, v, w]</td>
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<tr>
<td>z, 0, y [w, 0, v]</td>
<td>3/4, y, y + 1/2 [u, v, v]</td>
<td>y + 1/2, 3/4, y [v, u, v]</td>
<td>y + 1/2, 3/4, y [v, u, v]</td>
<td>0, y, z [0, v, w]</td>
<td></td>
</tr>
<tr>
<td>y, z, 0 [v, w, 0]</td>
<td>y + 1/2, 1/4 [v, u, v]</td>
<td>y + 1/2, 1/4 [v, u, v]</td>
<td>y + 1/2, 1/4 [v, u, v]</td>
<td>y + 1/2, 1/4 [v, u, v]</td>
<td></td>
</tr>
<tr>
<td>0, z, y [0, w, v]</td>
<td>3/4, y, y + 1/2 [u, v, v]</td>
<td>y + 1/2, 2/3, y [v, u, v]</td>
<td>y + 1/2, 2/3, y [v, u, v]</td>
<td>y + 1/2, 2/3, y [v, u, v]</td>
<td></td>
</tr>
<tr>
<td>z, y, 0 [w, v, 0]</td>
<td>y + 1/2, 2/4 [v, v, u]</td>
<td>y + 1/2, 2/4 [v, v, u]</td>
<td>y + 1/2, 2/4 [v, v, u]</td>
<td>y + 1/2, 2/4 [v, v, u]</td>
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<td>0, y, y [0, v, v]</td>
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<td>0, y, y [0, v, v]</td>
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<td>y, 0, y [v, 0, v]</td>
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<tr>
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<td>y, y, 0 [v, v, 0]</td>
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<td></td>
</tr>
<tr>
<td>0, 1/2, x [0, 0, u]</td>
<td>1/2, x, 0 [0, u, 0]</td>
<td>x, 1/2, x [0, 0, u]</td>
<td>x, 1/2, x [0, 0, u]</td>
<td>x, 1/2, x [0, 0, u]</td>
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<tr>
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<td>1/2, x, 0 [0, u, 0]</td>
<td>1/2, x, 0 [0, u, 0]</td>
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<tr>
<td>0, x, 0 [0, 0, u]</td>
<td>0, x, 0 [0, 0, u]</td>
<td>0, x, 0 [0, 0, u]</td>
<td>0, x, 0 [0, 0, u]</td>
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</tr>
<tr>
<td>x, x, x [u, u, u]</td>
<td>x, x, x [u, u, u]</td>
<td>x, x, x [u, u, u]</td>
<td>x, x, x [u, u, u]</td>
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<td>x, x, x [u, u, u]</td>
<td>x, x, x [u, u, u]</td>
<td>x, x, x [u, u, u]</td>
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</tbody>
</table>

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Symmetry of Special Projections

Along [0,0,1] p4'm'm
a* = (a - b)/2  b* = (a + b)/2
Origin at 0,0,z

Along [1,1,1] p6mm
a* = (2a - b - c)/3  b* = (-a + 2b - c)/3
Origin at x,x,x

Along [1,1,0] p2mm1*
a* = (-a + b)/2  b* = c/2
Origin at x,x,0

Continued
Origin at center (m3m')

**Asymmetric unit**

\[
0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y \leq x; \quad z \leq \min(1/2-x,y)
\]

**Vertices**

\[
0,0,0 \quad 1/2,0,0 \quad 1/2,1/2,0 \quad 1/4,1/4,1/4
\]

**Symmetry Operations**

<table>
<thead>
<tr>
<th>For (0,0,0) + set</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1 (1),0,0,0</td>
</tr>
<tr>
<td>(2) 2 0,0,z</td>
</tr>
<tr>
<td>(3) 2 0,y,0</td>
</tr>
<tr>
<td>(4) 2 x,0,0</td>
</tr>
<tr>
<td>(5) 3' x,x,x (3_{xyz}</td>
</tr>
<tr>
<td>(6) 3' x,x,x (3_{xyz}</td>
</tr>
<tr>
<td>(7) 3' x,x,x (3_{xyz}</td>
</tr>
<tr>
<td>(8) 3' x,x,x (3_{xyz}</td>
</tr>
<tr>
<td>(9) 3' x,x,x (3_{xyz}</td>
</tr>
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Continued

(33) $\bar{3}$ x,x,x; $1/4,1/4,1/4$
     (3$_{xy}$z) $1/2,1/2,1/2$
(34) $\bar{3}$ x+1,x-1,x; $1/4,-1/4,3/4$
     (3$_{xy}$z) $1/2,1/2,1/2$
(35) $\bar{3}$ x,x+1,x; $-1/4,3/4,1/4$
     (3$_{xy}$z) $1/2,1/2,1/2$
(36) $\bar{3}$ x+1,x,x; $3/4,1/4,-1/4$
     (3$_{xy}$z) $1/2,1/2,1/2$

(37) c' (0,0,1/2) x+1/2,x,z
     (m$_{yz}$) $1/2,1/2,1/2$
(38) n' (1/2,1/2,1/2) x,x,z
     (m$_{xy}$) $1/2,1/2,1/2$
(39) 4' - 0,1/2,z; 0,1/2,1/4
     (4'z) $1/2,1/2,1/2$
(40) 4' - 1/2,0,z; 1/2,0,1/4
     (4'z) $1/2,1/2,1/2$

(41) 4' x,0,1/2; 1/4,0,1/2
     (4'x) $1/2,1/2,1/2$
(42) a' (1/2,0,0) x+y+1/2,y
     (m$_{yz}$) $1/2,1/2,1/2$
(43) n' (1/2,1/2,1/2) x,y,y
     (m$_{yz}$) $1/2,1/2,1/2$
(44) 4' x,1/2,0; 1/4,1/2,0
     (4'x) $1/2,1/2,1/2$

(45) 4' 0,y,1/2; 0,1/4,1/2
     (4'y) $1/2,1/2,1/2$
(46) b' (0,1/2,0) x+1/2,y,x
     (m$_{xz}$) $1/2,1/2,1/2$
(47) 4' - 1/2,y,0; 1/2,1/4,0
     (4'y) $1/2,1/2,1/2$
(48) n' (1/2,1/2,1/2) x,y,x
     (m$_{xz}$) $1/2,1/2,1/2$

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

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<table>
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<tr>
<th></th>
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<th>Coordinates</th>
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<td>(2) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>(42) x,z,y [u,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>(46) z,y,x [w,v,u]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>x,x,z [u,u,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>z,x,x [w,u,u]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>x,x,x [u,u,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>x,x,x [u,w,u]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<td>x,x,x [u,u,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
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<tr>
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<td>x,x,x [u,w,u]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
<tr>
<td></td>
<td>x,x,x [u,w,u]</td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
</tr>
</tbody>
</table>
Continued

\[ z, x, x \ [w, u, u] \]

48 j m

\[ 0, y, z \ [u, 0, 0] \]

\[ 0, y, z \ [u, 0, 0] \]

\[ 0, y, z \ [u, 0, 0] \]

\[ 0, y, z \ [u, 0, 0] \]

\[ 0, y, z \ [u, 0, 0] \]

48 i ..

\[ 1/4, y, y + 1/2 \ [0, v, v] \]

\[ 3/4, y, y + 1/2 \ [0, v, v] \]

\[ 3/4, y, y + 1/2 \ [0, v, v] \]

\[ 1/4, y, y + 1/2 \ [0, v, v] \]

\[ 3/4, y, y + 1/2 \ [0, v, v] \]

\[ y + 1/2, 1/4 \ [v, 0, v] \]

\[ y + 1/2, 1/4 \ [v, 0, v] \]

\[ y + 1/2, 1/4 \ [v, 0, v] \]

\[ y + 1/2, 1/4 \ [v, 0, v] \]

\[ y + 1/2, 1/4 \ [v, 0, v] \]

24 h m.m'2

\[ 0, y, y \ [u, 0, 0] \]

\[ 0, y, y \ [u, 0, 0] \]

\[ 0, y, y \ [u, 0, 0] \]

\[ 0, y, y \ [u, 0, 0] \]

\[ 0, y, y \ [u, 0, 0] \]

24 g mm2

\[ x, 0, 1/2 \ [0, 0, 0] \]

\[ x, 0, 1/2 \ [0, 0, 0] \]

\[ 1/2, x, 0 \ [0, 0, 0] \]

\[ 1/2, x, 0 \ [0, 0, 0] \]

\[ 1/2, x, 0 \ [0, 0, 0] \]

16 f .3m'

\[ x, x, x \ [u, u, u] \]

\[ x, x, x \ [u, u, u] \]

\[ x, x, x \ [u, u, u] \]

\[ x, x, x \ [u, u, u] \]

\[ x, x, x \ [u, u, u] \]

12 e 4'm.m'

\[ x, 0, 0 \ [0, 0, 0] \]

\[ x, 0, 0 \ [0, 0, 0] \]

\[ 0, x, 0 \ [0, 0, 0] \]

\[ 0, x, 0 \ [0, 0, 0] \]

\[ 0, x, 0 \ [0, 0, 0] \]

12 d 4'm.2'

\[ 1/4, 0, 1/2 \ [0, 0, 0] \]

\[ 3/4, 0, 1/2 \ [0, 0, 0] \]

\[ 1/2, 3/4, 0 \ [0, 0, 0] \]

\[ 0, 1/2, 1/4 \ [0, 0, 0] \]

\[ 0, 1/2, 1/4 \ [0, 0, 0] \]

8 c .3m'

\[ 1/4, 1/4, 1/4 \ [u, u, u] \]

\[ 3/4, 3/4, 1/4 \ [u, u, u] \]

\[ 3/4, 1/4, 3/4 \ [u, u, u] \]

\[ 1/4, 3/4, 3/4 \ [u, u, u] \]

6 b 4'mm.m'

\[ 0, 1/2, 1/2 \ [0, 0, 0] \]

\[ 1/2, 0, 1/2 \ [0, 0, 0] \]

\[ 1/2, 1/2, 0 \ [0, 0, 0] \]

2 a m3m'

\[ 0, 0, 0 \ [0, 0, 0] \]

\[ 0, 0, 0 \ [0, 0, 0] \]

\[ 0, 0, 0 \ [0, 0, 0] \]

\[ 0, 0, 0 \ [0, 0, 0] \]
Symmetry of Special Projections

Along [0,0,1]  p4mm1'  
\[ a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \]
Origin at 0,0,z

Along [1,1,1]  p6' mm'  
\[ a^* = \frac{(2a - b - c)}{3} \quad b^* = \frac{(-a + 2b - c)}{3} \]
Origin at x,x,x

Along [1,1,0]  p2'mm'  
\[ a^* = \frac{c}{2} \quad b^* = \frac{(-a + b)}{2} \]
Origin at x,x,0
Origin at center (m'3'm')

Asymmetric unit
0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ x; z ≤ min(1/2-x,y)

Vertices
0,0,0 1/2,0,0 1/2,1/2,0 1/4,1/4,1/4

Symmetry Operations

For (0,0,0) + set

(1) 1
(1') 0,0,0

(5) 3' x,x,x
(3_{xyz} | 0,0,0)

(9) 3' x,x,x
(3_{xyz}^{-1} | 0,0,0)

(2) 2 0,0,z
(2') 0,0,0

(6) 3' x,x,x
(3_{xyz}^{-1} | 0,0,0)

(10) 3' x,x,x
(3_{xyz} | 0,0,0)

(3) 2 0,y,0
(3') 0,0,0

(7) 3' x,x,x
(3_{xyz}^{-1} | 0,0,0)

(11) 3' x,x,x
(3_{xyz} | 0,0,0)

(4) 2 x,0,0
(4') 0,0,0

(8) 3' x,x,x
(3_{xyz}^{-1} | 0,0,0)
Continued

For \((1/2,1/2,1/2) + \text{set}\)

\[
\begin{align*}
(13) & \quad 2 \ x,x,0 \\
\quad (2_{xy}) 0,0,0 & \\
(14) & \quad 2 \ x,x,0 \\
\quad (2_{xy}) 0,0,0 & \\
(15) & \quad 4^+ \ 0,0,z \\
\quad (4_{z') 1,0,0) & \\
(16) & \quad 4^+ \ 0,0,z \\
\quad (4_{z'} 0,0,0) & \\
(17) & \quad 4^+ \ x,0,0 \\
\quad (4_{x'} 0,0,0) & \\
(18) & \quad 2 \ 0,y,y \\
\quad (2_{yz} 0,0,0) & \\
(19) & \quad 2 \ 0,y,y \\
\quad (2_{yz} 0,0,0) & \\
(20) & \quad 4^+ \ x,0,0 \\
\quad (4_{x'} 0,0,0) & \\
(21) & \quad 4^+ \ 0,y,0 \\
\quad (4_{y'} 0,0,0) & \\
(22) & \quad 2 \ x,0,x \\
\quad (2_{xz} 0,0,0) & \\
(23) & \quad 4^+ \ 0,y,0 \\
\quad (4_{y'} 0,0,0) & \\
(24) & \quad 2 \ x,0,x \\
\quad (2_{xz} 0,0,0) & \\
(25) & \quad \bar{1}^i \ 0,0,0 \\
\quad (\bar{1}^i 0,0,0) & \\
\quad (26) & \quad m' \ x,y,0 \\
\quad (m_{yz} 0,0,0') & \\
(27) & \quad m' \ x,0,z \\
\quad (m_{yz} 0,0,0') & \\
(28) & \quad m' \ 0,y,z \\
\quad (m_{yz} 0,0,0') & \\
(29) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
\quad (30) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
(31) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
(32) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
(33) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
\quad (34) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
\quad (35) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
\quad (36) & \quad \bar{3}^+ \ x,x,x; 0,0,0 \\
\quad (\bar{3}_{xyz} 0,0,0') & \\
(37) & \quad m' \ x,x,z \\
\quad (m_{yz} 0,0,0') & \\
\quad (38) & \quad m' \ x,x,z \\
\quad (m_{yz} 0,0,0') & \\
\quad (39) & \quad m' \ x,x,z \\
\quad (m_{yz} 0,0,0') & \\
\quad (40) & \quad m' \ x,x,z \\
\quad (m_{yz} 0,0,0') & \\
(41) & \quad \bar{4}^+ \ x,0,0; 0,0,0 \\
\quad (\bar{4}_{x'} 0,0,0') & \\
\quad (42) & \quad m' \ x,y,y \\
\quad (m_{yz} 0,0,0') & \\
\quad (43) & \quad m' \ x,y,y \\
\quad (m_{yz} 0,0,0') & \\
\quad (44) & \quad m' \ x,y,y \\
\quad (m_{yz} 0,0,0') & \\
(45) & \quad \bar{4}^+ \ 0,y,0; 0,0,0 \\
\quad (\bar{4}_{y'} 0,0,0') & \\
\quad (46) & \quad m' \ x,y,x \\
\quad (m_{yz} 0,0,0') & \\
\quad (47) & \quad m' \ x,y,x \\
\quad (m_{yz} 0,0,0') & \\
\quad (48) & \quad m' \ x,y,x \\
\quad (m_{yz} 0,0,0') & \\
\quad & 229.5.1642 - 2 \text{-} 3877
\end{align*}
\]
Continued

(33) \( y, z, x \) [v, w, u]
(34) \( x + 1, x - 1, x \)
(35) \( x, x + 1, x \)
(36) \( x + 1, x, x \)

(37) \( x, 0, 1/2 \) x + 1/2, x, z
(38) \( n' (1/2, 1/2, 1/2) \) x, x, z
(39) \( n' (1/2, 1/2, 1/2) \) x, x, z
(40) \( 1/2, 0, z \) 1/2, 0, 1/4

(41) \( 4^{-1} \) x, 0, 1/2; 1/4, 0, 1/2
(42) \( 4^{-1} \) x, 0, 1/2; 1/4, 0, 1/2
(43) \( n' (1/2, 1/2, 1/2) \) x, y, y
(44) \( 4^{-1} \) x, 1/2, 0; 1/4, 1/2, 0

(45) \( 4^{-1} \) 0, y, 1/2; 0, 1/4, 1/2
(46) \( b' (0, 1/2, 0) x + 1/2, x, x \)
(47) \( 4^{-1} \) 1/2, y, 0; 1/2, 1/4, 0
(48) \( n' (1/2, 1/2, 1/2) x, y, x \)

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

96 1 1

Coordinates

(0,0,0) + (1/2,1/2,1/2) +

(1) x,y,z [u,v,w]  
(2) \( x, y, z [u, v, w] \)  
(3) \( x, y, z [u, v, w] \)  
(4) \( x, y, z [u, v, w] \)

(5) z,x,y [w,u,v]  
(6) \( z, x, y [w, u, v] \)  
(7) \( z, x, y [w, u, v] \)  
(8) \( z, x, y [w, u, v] \)

(9) y,z,x [v,w,u]  
(10) \( y, z, x [v, w, u] \)  
(11) \( y, z, x [v, w, u] \)  
(12) \( y, z, x [v, w, u] \)

(13) y,x,z [v,u,w]  
(14) \( y, x, z [v, u, w] \)  
(15) \( y, x, z [v, u, w] \)  
(16) \( y, x, z [v, u, w] \)

(17) x,y,z [u,w,v]  
(18) \( x, y, z [u, w, v] \)  
(19) \( x, y, z [u, w, v] \)  
(20) \( x, y, z [u, w, v] \)

(21) z,y,x [w,v,u]  
(22) \( z, y, x [w, v, u] \)  
(23) \( z, y, x [w, v, u] \)  
(24) \( z, y, x [w, v, u] \)

(25) x,y,z [u,v,w]  
(26) \( x, y, z [u, v, w] \)  
(27) \( x, y, z [u, v, w] \)  
(28) \( x, y, z [u, v, w] \)

(29) z,x,y [w,u,v]  
(30) \( z, x, y [w, u, v] \)  
(31) \( z, x, y [w, u, v] \)  
(32) \( z, x, y [w, u, v] \)

(33) y,z,x [v,w,u]  
(34) \( y, z, x [v, w, u] \)  
(35) \( y, z, x [v, w, u] \)  
(36) \( y, z, x [v, w, u] \)

(37) y,x,z [v,u,w]  
(38) \( y, x, z [v, u, w] \)  
(39) \( y, x, z [v, u, w] \)  
(40) \( y, x, z [v, u, w] \)

(41) x,z,y [u,w,v]  
(42) \( x, z, y [u, w, v] \)  
(43) \( x, z, y [u, w, v] \)  
(44) \( x, z, y [u, w, v] \)

(45) z,y,x [w,v,u]  
(46) \( z, y, x [w, v, u] \)  
(47) \( z, y, x [w, v, u] \)  
(48) \( z, y, x [w, v, u] \)

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<td>48 j m'</td>
<td>( z, x, x ) [( w, u, u )]</td>
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<td>48 i</td>
<td>..2</td>
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<td>24 h m'.m'2</td>
<td>( 3/4, y, y+1/2 ) [( 0, v, v )]</td>
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<td>24 g m'm'2</td>
<td>( y+1/2, 1/4, y ) [( v, 0, v )]</td>
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<tr>
<td>16 f .3m'</td>
<td>( x, x, x ) [( u, u, u )]</td>
</tr>
<tr>
<td>12 e 4m'.m'</td>
<td>( x, 0, 0 ) [( u, 0, 0 )]</td>
</tr>
<tr>
<td>12 d 4'm'.2</td>
<td>( 1/2, 3/4, 0 ) [( 0, 0, 0 )]</td>
</tr>
<tr>
<td>8 c .3'm'</td>
<td>( 1/4, 1/4, 1/4 ) [( 0, 0, 0 )]</td>
</tr>
<tr>
<td>6 b 4/m'm'.m'</td>
<td>( 0, 1/2, 1/2 ) [( 0, 0, 0 )]</td>
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<tr>
<td>2 a m'3'm'</td>
<td>( 0, 0, 0 ) [( 0, 0, 0 )]</td>
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Symmetry of Special Projections

<table>
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<tr>
<th>Direction</th>
<th>p4m' m'</th>
<th>p6m' m'</th>
<th>p2m' m'</th>
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<tbody>
<tr>
<td>[0,0,1]</td>
<td>(a^<em>= (a - b)/2) (b^</em>= (a + b)/2)</td>
<td>(a^<em>= (2a - b - c)/3) (b^</em>= (-a + 2b - c)/3)</td>
<td>(a^<em>= (-a + b)/2) (b^</em>= c/2)</td>
</tr>
<tr>
<td>Origin</td>
<td>0,0,z</td>
<td>x,x,x</td>
<td>x,x,0</td>
</tr>
</tbody>
</table>
Origin at center \((m\bar{3}m)\)

Asymmetric unit: \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y < x; \quad z \leq \min(1/2-x,y)\)

Vertices: \(0,0,0\); \(1/2,0,0\); \(1/2,1/2,0\); \(1/4,1/4,1/4\)

Symmetry Operations

For \((0,0,0) + \text{ set}\)

1. \(1\)
2. \(2 \quad 0,0,z\)
3. \(2 \quad 0,y,0\)
4. \(2 \quad x,0,0\)

5. \(3^+ \ x,x,x\)
6. \(3^+ \ x,x,x\)
7. \(3^+ \ x,x,x\)
8. \(3^+ \ x,x,x\)

9. \(3^{-} \ x,x,x\)
10. \(3^{-} \ x,x,x\)
11. \(3^{-} \ x,x,x\)
12. \(3^{-} \ x,x,x\)

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Continued

(33) $\bar{3}$: x,x,x; 
\[ \frac{1}{2}, \frac{1}{2}, 1/2 \] 
(34) $\bar{3}$: x+1, x-1, x; 
\[ \frac{1}{2}, \frac{1}{2}, 1/2 \] 
(35) $\bar{3}$: x, x+1, x; 
\[ \frac{1}{2}, \frac{1}{2}, 1/2 \] 
(36) $\bar{3}$: x+1, x, x; 
\[ \frac{1}{2}, \frac{1}{2}, 1/2 \] 

(37) c' (0,0,1/2) x+1/2, x, z 
\[ m_{xy} \] 1/2, 1/2, 1/2

(38) n' (1/2,1/2,1/2) x,x,z 
\[ m_{xy} \] 1/2, 1/2, 1/2

(39) 4' - 0,1/2,z; 0,1/2,1/4 
\[ 4' \] 1/2,1/2,1/2

(40) 4' - 1/2,0,z; 1/2,0,1/4 
\[ 4' \] 1/2,1/2,1/2

(41) 4' - x,0,1/2; 1/4,0,1/2 
\[ 4' \] 1/2,1/2,1/2

(42) a' (1/2,0,0) x,y+1/2, y 
\[ m_{yx} \] 1/2,1/2,1/2

(43) n' (1/2,1/2,1/2) x,y,y 
\[ m_{yx} \] 1/2,1/2,1/2

(44) 4' - 1/2,1/2,0; 1/4,1,2,0 
\[ 4' \] 1/2,1/2,1/2

(45) 4' - 0,y,1/2; 0,1/4,1/2 
\[ 4' \] 1/2,1/2,1/2

(46) b' (0,1/2,0) x+1/2,y,x 
\[ m_{xz} \] 1/2,1/2,1/2

(47) 4' - 1/2,y,0; 1/2,1/4,0 
\[ 4' \] 1/2,1/2,1/2

(48) n' (1/2,1/2,1/2) x,y,x 
\[ m_{xz} \] 1/2,1/2,1/2

Generators selected  (1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

96  l  1

(1) x,y,z [u,v,w]  (2) x,y,z [u,v,w]  (3) x,y,z [u,v,w]  (4) x,y,z [u,v,w]

(5) z,x,y [w,u,v]  (6) z,x,y [w,u,v]  (7) z,x,y [w,u,v]  (8) z,x,y [w,u,v]

(9) y,z,x [v,w,u]  (10) y,z,x [v,w,u]  (11) y,z,x [v,w,u]  (12) y,z,x [v,w,u]

(13) y,z,x [v,u,w]  (14) y,z,x [v,u,w]  (15) y,z,x [v,u,w]  (16) y,z,x [v,u,w]

(17) x,z,y [u,w,v]  (18) x,z,y [u,w,v]  (19) x,z,y [u,w,v]  (20) x,z,y [u,w,v]

(21) z,y,x [w,v,u]  (22) z,y,x [w,v,u]  (23) z,y,x [w,v,u]  (24) z,y,x [w,v,u]

(25) x,y,z [u,v,w]  (26) x,y,z [u,v,w]  (27) x,y,z [u,v,w]  (28) x,y,z [u,v,w]

(29) z,x,y [w,u,v]  (30) z,x,y [w,u,v]  (31) z,x,y [w,u,v]  (32) z,x,y [w,u,v]

(33) y,z,x [v,w,u]  (34) y,z,x [v,w,u]  (35) y,z,x [v,w,u]  (36) y,z,x [v,w,u]

(37) y,z,x [v,u,w]  (38) y,z,x [v,u,w]  (39) y,z,x [v,u,w]  (40) y,z,x [v,u,w]

(41) x,z,y [u,w,v]  (42) x,z,y [u,w,v]  (43) x,z,y [u,w,v]  (44) x,z,y [u,w,v]

(45) z,y,x [w,v,u]  (46) z,y,x [w,v,u]  (47) z,y,x [w,v,u]  (48) z,y,x [w,v,u]
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<tr>
<th>Column 1</th>
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<th>Column 3</th>
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<tr>
<td>48</td>
<td>j</td>
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<td>1/4,y,y +1/2</td>
<td>1/4,y,y +1/2</td>
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<td>x,x,x [0,0,0]</td>
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<tr>
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<td>e</td>
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<td>0,1/2,3/4 [0,0,0]</td>
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<td>3/4,1/4,3/4 [0,0,0]</td>
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<tr>
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</table>
Symmetry of Special Projections

Along [0,0,1]  p4mm1'
\( a^* = \frac{(a - b)}{2} \quad b^* = \frac{(a + b)}{2} \)
Origin at 0,0,z

Along [1,1,1]  p6mm1'
\( a^* = \frac{(2a - b - c)}{3} \quad b^* = \frac{(-a + 2b - c)}{3} \)
Origin at x,x,x

Along [1,1,0]  p2mm1'
\( a^* = \frac{(-a + b)}{2} \quad b^* = \frac{c}{2} \)
Origin at x,x,0
Origin at center (m\(^3\)\(^\prime\)m)

Asymmetric unit: 
- \(0 \leq x \leq 1/2; \quad 0 \leq y \leq 1/2; \quad 0 \leq z \leq 1/4; \quad y \leq x; \quad z \leq \min(1/2-x,y)

Vertices: 
- 0,0,0
- 1/2,0,0
- 1/2,1/2,0
- 1/4,1/4,1/4

Symmetry Operations

For \((0,0,0) + \text{set}\):

1. \(1\)
2. \(2\) \((0,0,z)\)
3. \(2\) \((0,y,0)\)
4. \(2\) \((x,0,0)\)

5. \(3^+ x,x,x\)
6. \(3^+ x,x,x\)
7. \(3^+ x,x,x\)
8. \(3^+ x,x,x\)

9. \(3^- x,x,x\)
10. \(3^- x,x,x\)
11. \(3^- x,x,x\)
12. \(3^- x,x,x\)
Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13); (25).

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
<tbody>
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<td>96</td>
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<table>
<thead>
<tr>
<th>Coordinates</th>
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<th>(1/2,1/2,1/2)' +</th>
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<tr>
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<td>(3) x, y, z [u,v,w]</td>
</tr>
<tr>
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<td>(17) x, y, z [w,v,u]</td>
<td>(18) x, y, z [w,v,u]</td>
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<td>(21) x, y, z [w,v,u]</td>
</tr>
<tr>
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<td>(23) x, y, z [w,v,u]</td>
<td>(24) x, y, z [w,v,u]</td>
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<td>(26) x, y, z [w,v,u]</td>
<td>(27) x, y, z [w,v,u]</td>
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<td>(31) z, x, y [w,u,v]</td>
<td>(32) z, x, y [w,u,v]</td>
<td>(33) y, z, x [v,w,u]</td>
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<tr>
<td>(34) y, z, x [v,w,u]</td>
<td>(35) y, z, x [v,w,u]</td>
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<td>(42) x, z, y [u,w,v]</td>
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<tr>
<td>(43) x, z, y [u,w,v]</td>
<td>(44) x, z, y [u,w,v]</td>
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<th>m'..</th>
<th>k</th>
<th>m'2..</th>
<th>l</th>
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<tbody>
<tr>
<td>48</td>
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<td>48</td>
<td>z,x,x [0, u, u]</td>
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<td>z,x,x [0, u, u]</td>
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<td>24</td>
<td>y, y [0, v, v]</td>
<td>24</td>
<td>y, y [0, v, v]</td>
<td>24</td>
<td>y, y [0, v, v]</td>
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<tr>
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<td>24</td>
<td>y, y [0, v, v]</td>
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<tr>
<td>0, z, y [0, w, v]</td>
<td>16</td>
<td>x, x, x [u, u, u]</td>
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<td>x, x, x [u, u, u]</td>
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<tr>
<td>12</td>
<td>4m'.m</td>
<td>x,0,0 [0, 0, 0]</td>
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</table>
Symmetry of Special Projections

Along \([0,0,1]\) \(p_4m'm'\)
\(a^* = (a - b)/2\) \(b^* = (a + b)/2\)
Origin at \(1/2,0,z\)

Along \([1,1,1]\) \(p6mm1'\)
\(a^* = (2a - b - c)/3\) \(b^* = (-a + 2b - c)/3\)
Origin at \(x,x,x\)

Along \([1,1,0]\) \(p2mm1'\)
\(a^* = (-a + b)/2\) \(b^* = c/2\)
Origin at \(x,x,0\)
Origin at center (m\text{3}m')

Asymmetric unit
0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/4; y \leq x; z \leq \min(1/2-x,y)

Vertices
0,0,0 1/2,0,0 1/2,1/2,0 1/4,1/4,1/4

Symmetry Operations
For (0,0,0) + set

(1) 1
(1) 0,0,0

(2) 2,0,0,z
(2) 0,0,0

(3) 2,0,y,0
(3) 0,0,0

(4) 2,x,0,0
(4) 0,0,0

(5) 3^+ x,x,x
(5) x,x,x
(3_{xyz}|0,0,0)

(6) 3^+ x,x,x
(6) x,x,x
(3_{xyz}^{-1}|0,0,0)

(7) 3^+ x,x,x
(7) x,x,x
(3_{xyz}^{-1}|0,0,0)

(8) 3^{-} x,x,x
(8) x,x,x
(3_{xyz}^{-1}|0,0,0)

(9) 3^+ x,x,x
(9) x,x,x
(3_{xyz}^{-1}|0,0,0)

(10) 3^+ x,x,x
(10) x,x,x
(3_{xyz}|0,0,0)

(11) 3^{-} x,x,x
(11) x,x,x
(3_{xyz}|0,0,0)

(12) 3^{-} x,x,x
(12) x,x,x
(3_{xyz}|0,0,0)
Continued

\[ (33) \vec{3}' \begin{array}{c} x, x, x \\ 1/4, 1/4, 1/4 \\ (\vec{3}_{xyz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (34) \vec{3}' \begin{array}{c} x+1, x-1, x \\ 1/4, -1/4, 3/4 \\ (\vec{3}_{xyz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (35) \vec{3}' \begin{array}{c} x, x+1, x \\ -1/4, 3/4, 1/4 \\ (\vec{3}_{xyz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (36) \vec{3}' \begin{array}{c} x+1, x, x \\ 3/4, 1/4, -1/4 \\ (\vec{3}_{xyz})^{1/2, 1/2, 1/2} \end{array} \]

\[ (37) c \begin{array}{c} (0,0,1/2) \\ x+1/2, x, z \\ (m_{yz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (38) n \begin{array}{c} (1/2, 1/2, 1/2) \\ x, x, z \\ (m_{yz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (39) 4^- \begin{array}{c} 0, 1/2, z \\ 1/2, 1/2, 1/2 \\ (m_{xz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (40) 4^- \begin{array}{c} 1/2, 0, z \\ 1/2, 0, 1/4 \\ (m_{xz})^{1/2, 1/2, 1/2} \end{array} \]

\[ (41) 4^- \begin{array}{c} x, 0, 1/2 \\ 1/4, 0, 1/2 \\ (4^x)^{1/2, 1/2, 1/2} \end{array} \]
\[ (42) a \begin{array}{c} (1/2, 0, 0) \\ y, x+1/2, y \\ (m_{yz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (43) n \begin{array}{c} (1/2, 1/2, 1/2) \\ x, y, y \\ (4^x)^{1/2, 1/2, 1/2} \end{array} \]

\[ (44) 4^- \begin{array}{c} x, 1/2, 0 \\ 1/4, 1/2, 0 \\ (4^x)^{1/2, 1/2, 1/2} \end{array} \]

\[ (45) 4^- \begin{array}{c} 0, y, 1/2 \\ 0, 1/4, 1/2 \\ (4_y)^{1/2, 1/2, 1/2} \end{array} \]
\[ (46) b \begin{array}{c} (0, 1/2, 0) \\ x+1/2, y, x \\ (m_{xz})^{1/2, 1/2, 1/2} \end{array} \]
\[ (47) 4^- \begin{array}{c} 1/2, y, 0 \\ 1/2, 1/4, 0 \\ (4^y)^{1/2, 1/2, 1/2} \end{array} \]
\[ (48) n \begin{array}{c} (1/2, 1/2, 1/2) \\ x, y, x \\ (m_{xz})^{1/2, 1/2, 1/2} \end{array} \]

Generators selected

\[ (1); (t(1,0,0); t(0,1,0); t(0,0,1); t'(1/2,1/2,1/2); (2); (3); (5); (13); (25). \]

Positions

Multiplicity,
Wyckoff letter,
Site Symmetry.

96 | l | 1

\[ (1) x, y, z \begin{array}{c} [u, v, w] \end{array} \]
\[ (5) z, x, y \begin{array}{c} [w, u, v] \end{array} \]
\[ (9) y, z, x \begin{array}{c} [v, w, u] \end{array} \]
\[ (13) y, z, x \begin{array}{c} [\bar{v}, u, w] \end{array} \]
\[ (17) x, z, y \begin{array}{c} [\bar{u}, w, v] \end{array} \]
\[ (21) z, y, x \begin{array}{c} [w, v, u] \end{array} \]
\[ (25) x, y, z \begin{array}{c} [u, v, w] \end{array} \]
\[ (29) z, x, y \begin{array}{c} [w, u, v] \end{array} \]
\[ (33) y, z, x \begin{array}{c} [v, w, u] \end{array} \]
\[ (37) y, z, x \begin{array}{c} [v, u, w] \end{array} \]
\[ (41) x, z, y \begin{array}{c} [u, w, v] \end{array} \]
\[ (45) z, y, x \begin{array}{c} [w, v, u] \end{array} \]

Coordinates

\[ (0,0,0) + (1/2,1/2,1/2)' + \]

229.8.1645 - 3 - 3893
Symmetry of Special Projections

Along [0,0,1]  p4mm1'  \[ a^* = (a - b)/2 \]  \[ b^* = (a + b)/2 \]
Origin at 0,0,z

Along [1,1,1]  p6mm1'  \[ a^* = (2a - b - c)/3 \]  \[ b^* = (-a + 2b - c)/3 \]
Origin at x,x,x

Along [1,1,0]  p2a* 2m'm'  \[ a^* = c/2 \]  \[ b^* = -(a + b)/2 \]
Origin at x,x,1/4
Origin at center (m'3'm')

Asymmetric unit: 0 ≤ x ≤ 1/2; 0 ≤ y ≤ 1/2; 0 ≤ z ≤ 1/4; y ≤ x; z ≤ min(1/2-x,y)

Vertices: 0,0,0, 1/2,0,0, 1/2,1/2,0, 1/4,1/2,1/4

Symmetry Operations:

For (0,0,0) + set

(1) 1
(1),0,0,0)

(2) 2 0,0,z
(2),0,0,0)

(3) 2 0,y,0
(2),0,0,0)

(4) 2 x,0,0
(2),0,0,0)

(9) 3+ x,x,x
(3*,0,0,0)

(6) 3* x,x,x
(3*,0,0,0)

(7) 3* x,x,x
(3*,0,0,0)

(8) 3* x,x,x
(3*,0,0,0)

(10) 3* x,x,x
(3*,0,0,0)

(11) 3* x,x,x
(3*,0,0,0)

(12) 3* x,x,x
(3*,0,0,0)
Continued

| (33) $\bar{3}$ | x,x,x; 1/4,1/2,1/2 | (34) $\bar{3}$ | x+1/2, x-1/2, x; 1/4,1/2,1/2 | (35) $\bar{3}$ | x,x,1; 1/4,1/4,1/4 | (36) $\bar{3}$ | x+1, x,x; 3/4,1/4,-1/4 |
| (3) $xyz$ | (1/2,1/2,1/2) | (3) $xyz$ | (1/2,1/2,1/2) | (3) $xyz$ | (1/2,1/2,1/2) | (3) $xyz$ | (1/2,1/2,1/2) |

| (37) c (0,0,1/2) | x+1/2, x,z; m,y | (38) n (1/2,1/2,1/2) | x,x,z; m,y | (39) $\bar{4}$ | 0,1/2; z, 0,1/2,1/4 | (40) $\bar{4}$ | 1/2,0,0; 1/2,0,1/4 |
| (5) $xyz$ | (1/2,1/2,1/2) | (5) $xyz$ | (1/2,1/2,1/2) | (4) $x^{-1}$ | 1/2,1/2,1/2 | (4) $x^{-1}$ | 1/2,1/2,1/2 |

| (41) $\bar{4}$ | x,0,1/2; 1/4,0,1/2 | (42) a (1/2,0,0) | x,y+1/2, y,z; m,y | (43) n (1/2,1/2,1/2) | x,y,y; m,y | (44) $\bar{4}$ | x,1/2,0; 1/4,1/2,0 |
| (5) $xyz$ | (1/2,1/2,1/2) | (5) $xyz$ | (1/2,1/2,1/2) | (4) $x^{-1}$ | 1/2,1/2,1/2 | (4) $x^{-1}$ | 1/2,1/2,1/2 |

| (45) $\bar{4}$ | 0,y,1/2; 0,1/4,1/2 | (46) b (0,1/2,0) | x+1/2, y,x; m,y | (47) $\bar{4}$ | 1/2,2,y; 0,1/2,1/4,0 | (48) n (1/2,1/2,1/2) | x,y,x; m,y |
| (4) $xyz$ | (1/2,1/2,1/2) | (4) $xyz$ | (1/2,1/2,1/2) | (4) $y^{-1}$ | 1/2,1/2,1/2 | (4) $y^{-1}$ | 1/2,1/2,1/2 |

Generators selected

1. (1,0,0); 2. (0,1,0); 3. (0,0,1); 4. (1/2,1,1/2); 5. (1/2,1,1/2); 6. (2); 7. (3,5); 8. (13); 9. (25).

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site Symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>96</td>
<td>l 1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Position</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) x,y,z [u,v,w]</td>
<td>(0,0,0) + (1/2,1/2,1/2)' +</td>
</tr>
<tr>
<td>(5) z,x,y [w,u,v]</td>
<td></td>
</tr>
<tr>
<td>(9) y,z,x [v,w,u]</td>
<td></td>
</tr>
<tr>
<td>(12) y,z,x [v,w,u]</td>
<td></td>
</tr>
<tr>
<td>(16) y,x,z [v,u,w]</td>
<td></td>
</tr>
<tr>
<td>(24) z,y,x [w,v,u]</td>
<td></td>
</tr>
<tr>
<td>(28) x,y,z [u,v,w]</td>
<td></td>
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<tr>
<td>(32) z,x,y [w,u,v]</td>
<td></td>
</tr>
<tr>
<td>(36) y,z,x [v,w,u]</td>
<td></td>
</tr>
<tr>
<td>(40) y,z,x [v,w,u]</td>
<td></td>
</tr>
<tr>
<td>(44) x,z,y [u,w,v]</td>
<td></td>
</tr>
<tr>
<td>(48) z,y,x [w,v,u]</td>
<td></td>
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Continued

<table>
<thead>
<tr>
<th>k</th>
<th>m'</th>
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<tr>
<td>48</td>
<td>x,x,z [u,u,w]</td>
</tr>
<tr>
<td>x,x,z [u,u,w]</td>
<td>x,x,z [u,u,w]</td>
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<td>x,x,z [u,u,w]</td>
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<td>x,z,x [w,u,u]</td>
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<tr>
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<td>x,z,x [w,u,u]</td>
</tr>
<tr>
<td>x,z,x [u,u,w]</td>
<td>x,z,x [u,u,w]</td>
</tr>
<tr>
<td>x,z,x [u,u,w]</td>
<td>x,z,x [u,u,w]</td>
</tr>
</tbody>
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229.9.1646 - 3 - 3898
<table>
<thead>
<tr>
<th>Column 1</th>
<th>Column 2</th>
<th>Column 3</th>
<th>Column 4</th>
<th>Column 5</th>
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<tbody>
<tr>
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<td>j</td>
<td>m'..</td>
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<tr>
<td>0, y, z</td>
<td>[0, v, w]</td>
<td>0, y, z</td>
<td>[0, v, w]</td>
<td>0, y, z</td>
</tr>
<tr>
<td>z, 0, y</td>
<td>[w, 0, v]</td>
<td>z, 0, y</td>
<td>[w, 0, v]</td>
<td>z, 0, y</td>
</tr>
<tr>
<td>y, 0, z</td>
<td>[v, 0, w]</td>
<td>y, 0, z</td>
<td>[v, 0, w]</td>
<td>y, 0, z</td>
</tr>
<tr>
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<td>[0, w, v]</td>
<td>0, y, z</td>
<td>[0, w, v]</td>
<td>0, y, z</td>
</tr>
<tr>
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<td>[w, v, 0]</td>
<td>z, y, 0</td>
<td>[w, v, 0]</td>
<td>z, y, 0</td>
</tr>
<tr>
<td>24</td>
<td>h</td>
<td>m'.m'2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0, y, y</td>
<td>[0, v, v]</td>
<td>0, y, y</td>
<td>[0, v, v]</td>
<td>0, y, y</td>
</tr>
<tr>
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<td>[v, 0, v]</td>
<td>y, 0, y</td>
<td>[v, 0, v]</td>
<td>y, 0, y</td>
</tr>
<tr>
<td>y, y, 0</td>
<td>[v, v, 0]</td>
<td>y, y, 0</td>
<td>[v, v, 0]</td>
<td>y, y, 0</td>
</tr>
<tr>
<td>24</td>
<td>g</td>
<td>m'm'2..</td>
<td>x, 0, 1/2</td>
<td>u, 0, 0</td>
</tr>
<tr>
<td>0, 1/2, x</td>
<td>[0, 0, u]</td>
<td>0, 1/2, x</td>
<td>[0, 0, u]</td>
<td>0, 1/2, x</td>
</tr>
<tr>
<td>x, 1/2, 0</td>
<td>[0, u, 0]</td>
<td>x, 1/2, 0</td>
<td>[0, u, 0]</td>
<td>x, 1/2, 0</td>
</tr>
<tr>
<td>16</td>
<td>f</td>
<td>.3m'</td>
<td>x, x, x</td>
<td>[u, u, u]</td>
</tr>
<tr>
<td>x, x, x</td>
<td>[u, u, u]</td>
<td>x, x, x</td>
<td>[u, u, u]</td>
<td>x, x, x</td>
</tr>
<tr>
<td>12</td>
<td>e</td>
<td>4m'.m'</td>
<td>x, 0, 0</td>
<td>[u, 0, 0]</td>
</tr>
<tr>
<td>x, 0, 0</td>
<td>[u, 0, 0]</td>
<td>x, 0, 0</td>
<td>[u, 0, 0]</td>
<td>x, 0, 0</td>
</tr>
<tr>
<td>0, x, 0</td>
<td>[0, u, 0]</td>
<td>0, x, 0</td>
<td>[0, u, 0]</td>
<td>0, x, 0</td>
</tr>
<tr>
<td>12</td>
<td>d</td>
<td>4m'.2'</td>
<td>1/4, 0, 1/2</td>
<td>u, 0, 0</td>
</tr>
<tr>
<td>1/2, 3/4, 0</td>
<td>[0, u, 0]</td>
<td>1/2, 3/4, 0</td>
<td>[0, u, 0]</td>
<td>1/2, 3/4, 0</td>
</tr>
<tr>
<td>8</td>
<td>c</td>
<td>.3m'</td>
<td>1/4, 1/4, 1/4</td>
<td>u, u, u</td>
</tr>
<tr>
<td>3/4, 3/4, 1/4</td>
<td>u, u, u</td>
<td>3/4, 1/4, 3/4</td>
<td>u, u, u</td>
<td>3/4, 1/4, 3/4</td>
</tr>
<tr>
<td>6</td>
<td>b</td>
<td>4/m'm'.m'</td>
<td>0, 1/2, 1/2</td>
<td>[0, 0, 0]</td>
</tr>
<tr>
<td>1/2, 0, 1/2</td>
<td>[0, 0, 0]</td>
<td>1/2, 0, 1/2</td>
<td>[0, 0, 0]</td>
<td>1/2, 0, 1/2</td>
</tr>
<tr>
<td>2</td>
<td>a</td>
<td>m'3'm'</td>
<td>0, 0, 0</td>
<td>[0, 0, 0]</td>
</tr>
</tbody>
</table>

229.9.1646 - 4 - 3899
Symmetry of Special Projections

Along \([0,0,1]\) \(p4mm1'\)
\[\mathbf{a}^* = (\mathbf{a} - \mathbf{b})/2 \quad \mathbf{b}^* = (\mathbf{a} + \mathbf{b})/2\]
Origin at 0,0,z

Along \([1,1,1]\) \(p6mm1'\)
\[\mathbf{a}^* = (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \quad \mathbf{b}^* = (\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3\]
Origin at x,x,x

Along \([1,1,0]\) \(p2mm1'\)
\[\mathbf{a}^* = (-\mathbf{a} + \mathbf{b})/2 \quad \mathbf{b}^* = \mathbf{c}/2\]
Origin at x,x,0
**Symmetry Operations**

For $(0,0,0) + \text{set}$

<table>
<thead>
<tr>
<th>(1)  $t$ $(1/2,1/2,1/2)$</th>
<th>(2)  $2 (0,0,1/2) 1/4,0,z$</th>
<th>(3)  $2 (0,1/2,0) 0,y,1/4$</th>
<th>(4)  $2 (1/2,0,0) x,1/4,0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1</td>
<td>0,0,0)$</td>
<td>$(2_z</td>
<td>1/2,0,1/2)$</td>
</tr>
<tr>
<td>(5)  $3^+$ $x,x,x$</td>
<td>(6)  $3^- x+1/2,x,-x$</td>
<td>(7)  $3^+ x+1/2,-x+1/2, x$</td>
<td>(8)  $3^+ x,-x+1/2, x$</td>
</tr>
<tr>
<td>$(3_{xyz}</td>
<td>0,0,0)$</td>
<td>$(3_{xyz}^{-1}</td>
<td>1/2,1/2,0)$</td>
</tr>
<tr>
<td>(9)  $3^- x,x,x$</td>
<td>(10)  $3^- (-1,3,1/3,1/3)$ $x+1/6,x+1/6,x$</td>
<td>(11)  $3^- (1,3,1/3,1/3)$ $x+1/3,x+1/3,x$</td>
<td>(12)  $3^- (1,-3,1/3,1/3)$ $x-1/6,x+1/3,x$</td>
</tr>
<tr>
<td>$(3_{xyz}^{-1}</td>
<td>0,0,0)$</td>
<td>$(3_{xyz}^{-1}</td>
<td>1/2,1/2,0)$</td>
</tr>
</tbody>
</table>

For $(1/2,1/2,1/2) + \text{set}$

<table>
<thead>
<tr>
<th>(1)  $t$ $(1/2,1/2,1/2)$</th>
<th>(2)  $2 (0,1/4,z)$</th>
<th>(3)  $2 (1/4,y,0)$</th>
<th>(4)  $2 (x,0,1/4)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1</td>
<td>1/2,1/2,1/2)$</td>
<td>$(2_z</td>
<td>1/2,0,1/2)$</td>
</tr>
<tr>
<td>(5)  $3^+$ $(1/2,1/2,1/2)$ $x,x,x$</td>
<td>(6)  $3^- (1/6,-1/6,1/6)$ $x-1/6,x+1/3,x,x$</td>
<td>(7)  $3^- (-1/6,1/6,1/6)$ $x+1/6,x+1/6,x,x$</td>
<td>(8)  $3^+ (1/6,1/6,-1/6)$ $x+1/3,x+1/6,x,x$</td>
</tr>
<tr>
<td>$(3_{xyz}</td>
<td>1/2,1/2,1/2)$</td>
<td>$(3_{xyz}^{-1}</td>
<td>0,0,1/2)$</td>
</tr>
</tbody>
</table>
Continued

Generators selected  
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

Positions

Coordinates

96   h   1

(0,0,0) + (1/2,1/2,1/2) +

(1) x,y,z [u,v,w]  
(2) x+1/2,y,z+1/2 [u,v,w]  
(3) x,y+1/2,z+1/2 [u,v,w]  
(4) x+1/2,y+1/2,z [u,v,w]  

(5) z,x,y [w,u,v]  
(6) z+1/2,x+1/2,y [w,u,v]  
(7) z+1/2,x,y+1/2 [w,u,v]  
(8) z,x+1/2,y+1/2 [w,u,v]  

(9) y,z,x [v,w,u]  
(10) y,z+1/2,x+1/2 [v,w,u]  
(11) y+1/2,z+1/2,x [v,w,u]  
(12) y+1/2,z+1/2 [v,w,u]  

(13) y+3/4,x+1/4,z+1/4 [v,u,w]  
(14) y+3/4,x+3/4,z+3/4 [v,u,w]  
(15) y+1/4,x+1/4,z+3/4 [v,u,w]  
(16) y+1/4,x+3/4,z+1/4 [v,u,w]  

(17) x+3/4,z,1/2,y+3/4 [u,w,v]  
(18) x+1/4,z+1/4,y+1/4 [u,w,v]  
(19) x+3/4,z+3/4,y+3/4 [u,w,v]  
(20) x+1/4,z+1/4,y+3/4 [u,w,v]  

(21) z+3/4,y+1/4,x+1/4 [w,v,u]  
(22) z+1/4,y+3/4,x+1/4 [w,v,u]  
(23) z+1/4,y+3/4,x+3/4 [w,v,u]  
(24) z+3/4,y+3/4,x+3/4 [w,v,u]  

(25) x,y,z [u,v,w]  
(26) x+1/2,y,z+1/2 [u,v,w]  
(27) x,y+1/2,z+1/2 [u,v,w]  
(28) x+1/2,y+1/2,z [u,v,w]
Continued 230.1.1647

(29) \( z, x, y \) [w, u, v]  
(30) \( z+1/2, x+1/2, y \) [w, u, v]  
(31) \( z+1/2, x, y+1/2 \) [w, u, v]  
(32) \( z, x+1/2, y+1/2 \) [w, u, v]  
(33) \( y, z, x \) [v, w, u]  
(34) \( y, z+1/2, x+1/2 \) [v, w, u]  
(35) \( y+1/2, z+1/2, x \) [v, w, u]  
(36) \( y+1/2, z, x+1/2 \) [v, w, u]  
(37) \( y+1/4, x+3/4, z+3/4 \) [v, u, w]  
(38) \( y+1/4, x+1/4, z+1/4 \) [v, u, w]  
(39) \( y+3/4, x+3/4, z+1/4 \) [v, u, w]  
(40) \( y+3/4, x+1/4, z+3/4 \) [v, u, w]  
(41) \( x+1/4, z+3/4, y+3/4 \) [w, v, u]  
(42) \( x+3/4, z+1/4, y+3/4 \) [w, v, u]  
(43) \( x+1/4, z+1/4, y+1/4 \) [w, v, u]  
(44) \( x+3/4, z+3/4, y+1/4 \) [w, v, u]  
(45) \( z+1/4, y+3/4, x+1/4 \) [w, v, u]  
(46) \( z+3/4, y+3/4, x+1/4 \) [w, v, u]  
(47) \( z+3/4, y+1/4, x+3/4 \) [w, v, u]  
(48) \( z+1/4, y+1/4, x+1/4 \) [w, v, u]  

48 g  2

1/8, y, y+1/4 [0, v, v]  
3/8, y, y+3/4 [0, v, v]  
7/8, y+1/2, y+1/4 [0, v, v]  
5/8, y+1/2, y+3/4 [0, v, v]  

y+1/4, 1/8, y [v, 0, v]  
y+3/4, 3/8, y [v, 0, v]  
y+1/4, 7/8, y+1/2 [v, 0, v]  
y+3/4, 5/8, y+1/2 [v, 0, v]  

y, y+1/4, 1/8 [v, v, 0]  
y, y+3/4, 3/8 [v, v, 0]  
y+1/2, y+1/4, 7/8 [v, v, 0]  
y+1/2, y+3/4, 5/8 [v, v, 0]  

7/8, y, y+3/4 [0, v, v]  
5/8, y+1/4 [0, v, v]  
1/8, y+1/2, y+3/4 [0, v, v]  
3/8, y+1/2, y+1/4 [0, v, v]  

y+3/4, 7/8, y [v, 0, v]  
y+1/4, 5/8, y [v, 0, v]  
y+3/4, 1/8, y+1/2 [v, 0, v]  
y+1/4, 3/8, y+1/2 [v, 0, v]  

y, y+3/4, 7/8 [v, v, 0]  
y, y+1/4, 5/8 [v, v, 0]  
y+1/2, y+3/4, 1/8 [v, v, 0]  
y+1/2, y+1/4, 3/8 [v, v, 0]  

48 f  2

x, 0, 1/4 [u, 0, 0]  
x+1/2, 0, 3/4 [u, 0, 0]  
0, 1/4, x [0, 0, u]  
0, 3/4, x+1/2 [0, 0, u]  
3/4, x+1/4, 0 [0, u, 0]  
3/4, x+3/4, 1/2 [0, u, 0]  
x+3/4, 1/2, 1/4 [u, 0, 0]  
x+1/4, 0, 1/4 [u, 0, 0]  
0, 4/3, x+1/4, 0 [0, u, 0]  
1/2, 1/4, x+3/4 [0, 0, u]  

x, 0, 3/4 [u, 0, 0]  
x+1/2, 0, 1/4 [u, 0, 0]  
3/4, x, 0 [0, 0, u]  
1/4, x+1/4, 0 [0, u, 0]  
0, 3/4, x [0, 0, u]  
0, 1/4, x+1/2 [0, u, 0]  
1/4, x+3/4, 0 [0, u, 0]  
1/4, x+1/4, 1/2 [0, u, 0]  

x+1/4, 1/2, 3/4 [u, 0, 0]  
x+3/4, 0, 3/4 [u, 0, 0]  
0, 3/4, x+3/4 [0, u, 0]  
1/2, 3/4, x+1/4 [0, u, 0]  

32 e  3

x, x, x [u, u, u]  
x+1/2, x, x+1/2 [u, u, u]  
x, x+1/2, x+1/2 [u, u, u]  
x+1/2, x+1/2, x [u, u, u]  

x+3/4, x+1/4, x+1/4 [u, u, u]  
x+3/4, x+3/4, x+3/4 [u, u, u]  
x+1/4, x+1/4, x+3/4 [u, u, u]  
x+1/4, x+3/4, x+1/4 [u, u, u]  

x, x, x [u, u, u]  
x+1/2, x, x+1/2 [u, u, u]  
x, x+1/2, x+1/2 [u, u, u]  
x+1/2, x+1/2, x [u, u, u]  

x+1/4, x+3/4, x+3/4 [u, u, u]  
x+1/4, x+1/4, x+1/4 [u, u, u]  
x+3/4, x+3/4, x+1/4 [u, u, u]  
x+3/4, x+1/4, x+3/4 [u, u, u]  

12 d  4

3/8, 0, 1/4 [u, 0, 0]  
1/8, 0, 3/4 [u, 0, 0]  
1/4, 3/8, 0 [0, u, 0]  
3/4, 1/8, 0 [0, u, 0]  
0, 1/4, 3/8 [0, 0, u]  
0, 3/4, 1/8 [0, 0, u]  
3/4, 5/8, 0 [0, u, 0]  
3/4, 3/8, 1/2 [0, u, 0]  
1/8, 1/2, 1/4 [u, 0, 0]  
7/8, 0, 1/4 [u, 0, 0]  
0, 1/4, 7/8 [0, u, 0]  
1/2, 1/4, 1/8 [0, u, 0]  

24 c  2, 22

1/8, 0, 1/4 [0, 0, 0]  
3/8, 0, 3/4 [0, 0, 0]  
1/4, 1/8, 0 [0, 0, 0]  
3/4, 3/8, 0 [0, 0, 0]  
0, 1/4, 1/8 [0, 0, 0]  
0, 3/4, 3/8 [0, 0, 0]  
7/8, 0, 3/4 [0, 0, 0]  
5/8, 0, 1/4 [0, 0, 0]  
3/4, 7/8, 0 [0, 0, 0]  
1/4, 5/8, 0 [0, 0, 0]  
0, 3/4, 7/8 [0, 0, 0]  
0, 1/4, 5/8 [0, 0, 0]  

230.1.1647 - 4 - 3904
Symmetry of Special Projections

Along [0,0,1] p\textsubscript{4}m'm'
\begin{align*}
\mathbf{a}^* &= \mathbf{a}/2 \\
\mathbf{b}^* &= \mathbf{b}/2
\end{align*}
Origin at 1/4,0,z

Along [1,1,1] p\textsubscript{6'}m'm
\begin{align*}
\mathbf{a}^* &= (2\mathbf{a} - \mathbf{b} - \mathbf{c})/3 \\
\mathbf{b}^* &= (-\mathbf{a} + 2\mathbf{b} - \mathbf{c})/3
\end{align*}
Origin at x,x,x

Along [1,1,0] c\textsubscript{2}m'm'
\begin{align*}
\mathbf{a}^* &= (-\mathbf{a} + \mathbf{b})/2 \\
\mathbf{b}^* &= \mathbf{c}/2
\end{align*}
Origin at x,x+1/4,1/8
Origin at center \((\bar{3}1')\)

Asymmetric unit
\[-1/8 < x < 1/8; \quad -1/8 < y < 1/8; \quad 0 < z < 1/4; \quad \text{max}(x-x, y-y) < z\]

Vertices
<table>
<thead>
<tr>
<th>(x, y, z)</th>
<th>(1/8,1/8,1/8)</th>
<th>(-1/8,1/8,1/8)</th>
<th>(-1/8,-1/8,1/8)</th>
<th>(1/8,-1/8,1/8)</th>
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<th>(-1/8,-1/8,1/4)</th>
<th>(1/8,-1/8,1/4)</th>
</tr>
</thead>
</table>

Symmetry Operations

For \((0,0,0)\) + set

\(\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 (0,0,1/2) \\
(3) & \quad 2 (0,1/2,0) \\
(4) & \quad 2 (1/2,0,0) \\
(5) & \quad 3^+ x,x,x \\
(6) & \quad 3^+ x+1/2,x,x \\
(7) & \quad 3^+ x+1/2,x-1/2,x \\
(8) & \quad 3^+ \bar{x},x+1/2,x \\
(9) & \quad 3^+ x,x,x \\
(10) & \quad 3^+ (-1/3,1/3,1/3) \\
(11) & \quad 3^+ (1/3,1/3,-1/3) \\
(12) & \quad 3^+ (1/3,-1/3,1/3) \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
(13) & \quad 2 (1/2,1/2,0) \\
(14) & \quad 2 (1/2,1/2,1/2) \\
(15) & \quad 4^* (0,0,3/4) \\
(16) & \quad 4^* (0,0,1/4) \\
(17) & \quad 4^* (3/4,0,0) \\
(18) & \quad 4^* (3/4,3/4,3/4) \\
(19) & \quad 4^* (3/4,3/4,3/4) \\
(20) & \quad 4^* (3/4,3/4,3/4) \\
(21) & \quad 4^* (1/2,0,1/2) \\
(22) & \quad 4^* (1/2,0,1/2) \\
(23) & \quad 4^* (0,3/4,0) \\
(24) & \quad 4^* (0,3/4,0) \\
(25) & \quad \bar{1} 0,0,0 \\
(26) & \quad a (1/2,0,0) \\
(27) & \quad c (0,0,1/2) \\
(28) & \quad b (0,1/2,0) \\
(29) & \quad \bar{3}^* x,x,x; 0,0,0 \\
(30) & \quad \bar{3}^* \bar{x}-1/2,x+1,\bar{x}; \\
(31) & \quad \bar{3}^* x+1/2,\bar{x}+1/2,\bar{x}; \\
(32) & \quad \bar{3}^* \bar{x}+1,\bar{x}+1,\bar{x}; \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
(33) & \quad 3^* x,x,x; 0,0,0 \\
(34) & \quad 3^* x+1/2,x+1/2,\bar{x}; 0,0,1/2 \\
(35) & \quad 3^* \bar{x},x+1/2,x; 0,1/2,0 \\
(36) & \quad 3^* x+1/2,x,x; 1/2,0,0 \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
(37) & \quad d (-1/4,1/4,1/4) \\
(38) & \quad d (1/4,1/4,1/4) \\
(39) & \quad d (1/4,1/4,1/4) \\
(40) & \quad d (1/4,1/4,1/4) \\
(41) & \quad \bar{4}^* x,0,3/4; 1/8,0,3/4 \\
(42) & \quad \bar{4}^* x,0,3/4; 1/8,0,3/4 \\
(43) & \quad \bar{4}^* x,0,3/4; 1/8,0,3/4 \\
(44) & \quad \bar{4}^* x,0,3/4; 1/8,0,3/4 \\
(45) & \quad \bar{4}^* -1/4,y,1/2; -1/4,3/8,1/2 \\
(46) & \quad \bar{4}^* -1/4,y,1/2; -1/4,3/8,1/2 \\
(47) & \quad \bar{4}^* -1/4,y,1/2; -1/4,3/8,1/2 \\
(48) & \quad \bar{4}^* -1/4,y,1/2; -1/4,3/8,1/2 \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
(1) & \quad t (1/2,1/2,1/2) \\
(2) & \quad t (1/2,1/2,1/2) \\
(3) & \quad t (1/2,1/2,1/2) \\
(4) & \quad t (1/2,1/2,1/2) \\
(5) & \quad 3^* (1/2,1/2,1/2) \\
(6) & \quad 3^* (-1/6,1/6,1/6) \\
(7) & \quad 3^* (1/6,1/6,1/6) \\
(8) & \quad 3^* (1/6,1/6,1/6) \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
(3_{xyz})^{-1} & \quad 0,0,0 \\
\end{align*}\)

For \((1/2,1/2,1/2)\) + set

\(\begin{align*}
(1) & \quad 1 \\
(2) & \quad 2 (0,1/4,z) \\
(3) & \quad 2 (0,1/4,z) \\
(4) & \quad 2 (0,1/4,z) \\
(5) & \quad 3^* (1/2,1/2,1/2) \\
(6) & \quad 3^* (1/2,1/2,1/2) \\
(7) & \quad 3^* (1/2,1/2,1/2) \\
(8) & \quad 3^* (1/2,1/2,1/2) \\
(3_{xyz})^{-1} & \quad 0,0,1/2 \\
(3_{xyz})^{-1} & \quad 0,0,1/2 \\
(3_{xyz})^{-1} & \quad 0,0,1/2 \\
(3_{xyz})^{-1} & \quad 0,0,1/2 \\
\end{align*}\)
Continued

**Generators selected**
(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25); 1'.

**Positions**

<table>
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<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site Symmetry</th>
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</thead>
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<td>96</td>
<td>h</td>
<td>11'</td>
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<table>
<thead>
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<th>(0,0,0)</th>
<th>(1/2,1/2,1/2)</th>
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<td>(1/2,1/2,1/2) +</td>
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<tbody>
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<td>(1) x,y,z [0,0,0]</td>
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<tr>
<td>(2) x+1/2, y+1/2, z [0,0,0]</td>
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<tr>
<td>(3) x+y+1/2, z+1/2 [0,0,0]</td>
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<tr>
<td>(4) x+1/2, y+1/2, z [0,0,0]</td>
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<tr>
<td>(5) z+1/2, x+1/2, y [0,0,0]</td>
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<tr>
<td>(6) z+1/2, x+1/2, y+1/2 [0,0,0]</td>
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<td>(7) z+1/2, x+1/2, y [0,0,0]</td>
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<td>(8) z+1/2, x+1/2, y+1/2 [0,0,0]</td>
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<td>(48) y+1/2, z [0,0,0]</td>
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| (1/2,1/2,1/2) |
| (1/2,1/2,1/2) |

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<tr>
<td>7/8,y+1/4 [0,0,0]</td>
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<tr>
<td>5/8,y+1/4 [0,0,0]</td>
</tr>
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<td>y+1/4,1/8,y [0,0,0]</td>
</tr>
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| (0,0,0)     |
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| (1/2,1/2,1/2) |
| (1/2,1/2,1/2) |

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<p>| 230.2.1648 - 5 - 3910 |</p>
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<td>x + 3/4, x + 1/4, x + 1/4 [0, 0, 0]</td>
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</tr>
<tr>
<td>3/8, 0, 1/4 [0, 0, 0]</td>
<td>1/8, 0, 3/4 [0, 0, 0]</td>
<td>1/4, 3/8, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>0, 1/4, 3/8 [0, 0, 0]</td>
<td>0, 3/4, 1/8 [0, 0, 0]</td>
<td>3/4, 5/8, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>1/8, 1/2, 1/4 [0, 0, 0]</td>
<td>7/8, 0, 1/4 [0, 0, 0]</td>
<td>0, 1/4, 7/8 [0, 0, 0]</td>
</tr>
<tr>
<td>24</td>
<td>c</td>
<td>2.221'</td>
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<tr>
<td>1/8, 0, 1/4 [0, 0, 0]</td>
<td>3/8, 0, 3/4 [0, 0, 0]</td>
<td>1/4, 1/8, 0 [0, 0, 0]</td>
</tr>
<tr>
<td>0, 1/4, 1/8 [0, 0, 0]</td>
<td>0, 3/4, 3/8 [0, 0, 0]</td>
<td>7/8, 0, 3/4 [0, 0, 0]</td>
</tr>
<tr>
<td>3/4, 7/8, 0 [0, 0, 0]</td>
<td>1/4, 5/8, 0 [0, 0, 0]</td>
<td>0, 3/4, 7/8 [0, 0, 0]</td>
</tr>
<tr>
<td>16</td>
<td>b</td>
<td>.321'</td>
</tr>
<tr>
<td>-----</td>
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<td></td>
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<tr>
<td>1/8, 1/8, 1/8 [0, 0, 0]</td>
<td>3/8, 7/8, 5/8 [0, 0, 0]</td>
<td>7/8, 5/8, 3/8 [0, 0, 0]</td>
</tr>
<tr>
<td>7/8, 7/8, 7/8 [0, 0, 0]</td>
<td>5/8, 1/8, 3/8 [0, 0, 0]</td>
<td>1/8, 3/8, 5/8 [0, 0, 0]</td>
</tr>
<tr>
<td>16</td>
<td>a</td>
<td>.3.1'</td>
</tr>
<tr>
<td>-----</td>
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<td></td>
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</tr>
<tr>
<td>0, 0, 0 [0, 0, 0]</td>
<td>1/2, 0, 1/2 [0, 0, 0]</td>
<td>0, 1/2, 1/2 [0, 0, 0]</td>
</tr>
<tr>
<td>3/4, 1/4, 1/4 [0, 0, 0]</td>
<td>3/4, 3/4, 3/4 [0, 0, 0]</td>
<td>1/4, 1/4, 3/4 [0, 0, 0]</td>
</tr>
</tbody>
</table>

### Symmetry of Special Projections

- **Along [0, 0, 1]**: p4mm 1' (\(a^* = a/2\), \(b^* = b/2\), origin at 1/4, 0, z)  
- **Along [1, 1, 1]**: p6mm 1' (\(a^* = (2a - b - c)/3\), \(b^* = (-a + 2b - c)/3\), origin at x, x, x)  
- **Along [1, 1, 0]**: c2mm 1' (\(a^* = (-a + b)/2\), \(b^* = c/2\), origin at x, x + 1/4, 1/8)
Ia'3'd
230.3.1649

m'3'm

Cubic

l41/a'3'2/d
Origin at center \( (\overline{3}) \)

**Asymmetric unit**: 
- \(-1/8 \leq x \leq 1/8; \)  
- \(-1/8 \leq y \leq 1/8; \)  
- \(0 \leq z \leq 1/4; \)  
- \(\max(x,-x,y,-y) \leq z\)

**Vertices**:
- \((0,0,0)\)  
- \((1/8,1/8,1/8)\)  
- \((-1/8,1/8,1/8)\)  
- \((-1/8,-1/8,1/8)\)

**Symmetry Operations**

For \((0,0,0)\) + set

<table>
<thead>
<tr>
<th>(1) 1</th>
<th>(2) 2</th>
<th>(3) 3</th>
<th>(4) 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0,0,0))</td>
<td>((0,0,1/2))</td>
<td>((0,1/2,0))</td>
<td>((1/2,0,0))</td>
</tr>
<tr>
<td>((1,0,0))</td>
<td>((2,0,1/2))</td>
<td>((0,1/2,1))</td>
<td>((1/2,1,0))</td>
</tr>
<tr>
<td>((3,0,0))</td>
<td>((3,0,1/2))</td>
<td>((0,1/2,1))</td>
<td>((1/2,1,0))</td>
</tr>
</tbody>
</table>

\(\bar{x} = x+1/2, x, x\)

<table>
<thead>
<tr>
<th>(5) 3' x,x,x</th>
<th>(6) 3' (x+1/2, x, x)</th>
<th>(7) 3' (x+1/2, -x+1/2, x)</th>
<th>(8) 3' (x, x+1/2, x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((3,0,0))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
</tr>
<tr>
<td>((1,1,0))</td>
<td>((1,1,1))</td>
<td>((1,1,1))</td>
<td>((1,1,1))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(9) 3' x,x,x</th>
<th>(10) 3' ((-1/3,1/3,1/3)) x+1/6, x+1/6, x</th>
<th>(11) 3' ((-1/3,1/3,1/3)) x+1/6, x+1/6, x</th>
<th>(12) 3' ((-1/3,1/3,1/3)) x+1/6, x+1/6, x</th>
</tr>
</thead>
<tbody>
<tr>
<td>((3,0,0))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
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<tr>
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<td>((0,1,1))</td>
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</table>

**Symmetry Operations**

For \((1/2,1/2,1/2)\) + set

<table>
<thead>
<tr>
<th>(1) t</th>
<th>(2) 2</th>
<th>(3) 2</th>
<th>(4) 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>((1/2,1/2,1/2))</td>
<td>((0,1/4,z))</td>
<td>((1/4,0,y))</td>
<td>((x,0,1/4))</td>
</tr>
<tr>
<td>((1/2,1/2,1/2))</td>
<td>((0,1/4,z))</td>
<td>((1/4,0,y))</td>
<td>((x,0,1/4))</td>
</tr>
</tbody>
</table>

\(\bar{x} = -x+1/2, -x+1, x\)

<table>
<thead>
<tr>
<th>(5) 3' x,x,x</th>
<th>(6) 3' ((-1/6,1/6,1/6)) x-1/6, x+1/3, x</th>
<th>(7) 3' ((-1/6,1/6,1/6)) x+1/6, x+1/6, x</th>
<th>(8) 3' ((-1/6,1/6,1/6)) x+1/6, x+1/6, x</th>
</tr>
</thead>
<tbody>
<tr>
<td>((3,0,0))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
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<tr>
<td>((0,1,0))</td>
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<td>((0,1,1))</td>
<td>((0,1,1))</td>
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</table>

**Symmetry Operations**

For \((1/2,1/2,1/2)\) + set

<table>
<thead>
<tr>
<th>(1) t</th>
<th>(2) 2</th>
<th>(3) 2</th>
<th>(4) 2</th>
</tr>
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<tbody>
<tr>
<td>((1/2,1/2,1/2))</td>
<td>((0,1/4,z))</td>
<td>((1/4,0,y))</td>
<td>((x,0,1/4))</td>
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<tr>
<td>((1/2,1/2,1/2))</td>
<td>((0,1/4,z))</td>
<td>((1/4,0,y))</td>
<td>((x,0,1/4))</td>
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</table>

\(\bar{x} = x+1/2, x, x\)

<table>
<thead>
<tr>
<th>(5) 3' x,x,x</th>
<th>(6) 3' ((-1/6,1/6,1/6)) x-1/6, x+1/3, x</th>
<th>(7) 3' ((-1/6,1/6,1/6)) x+1/6, x+1/6, x</th>
<th>(8) 3' ((-1/6,1/6,1/6)) x+1/6, x+1/6, x</th>
</tr>
</thead>
<tbody>
<tr>
<td>((3,0,0))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
<td>((3,0,1/2))</td>
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<tr>
<td>((0,1,0))</td>
<td>((0,1,1))</td>
<td>((0,1,1))</td>
<td>((0,1,1))</td>
</tr>
<tr>
<td>Generators selected</td>
<td>Coordinates</td>
<td></td>
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<tr>
<td></td>
<td>(0,0,0) + (1/2,1/2,1/2) +</td>
<td></td>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity, Wyckoff letter, Site Symmetry.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>96 h 1</td>
</tr>
</tbody>
</table>

| (9) 3' (1/2,1/2,1/2) x,x,x | (10) 3' (1/6,-1/6,-1/6) x+1/6,x+1/6,x | (11) 3' (-1/6,-1/6,1/6) x+1/3,x+1/6,x | (12) 3' (-1/6,1/6,-1/6) x+1/6,x+1/3,x |
| (13) 2' (1/2,1/2,0) x,x+1/4,3/8 | (14) 2' x,x+1/4,1/8 | (15) 4' (0,0,1/4) 3/4,0,0 | (16) 4' (0,0,1/4) 1/4,1/2,z |
| (17) 4' (1/4,0,0) x,3/4,0 | (18) 2' (0,1/2,1/2) 3/8,y-1/4,y | (19) 2' (1/2,1/2,y) | (20) 4' (3/4,0,0) x,1/4,1/2 |
| (21) 4' (0,3/4,0) 1/2,y,1/4 | (20) 4' (0,1/2,0) 0,y,3/4 | (21) 4' (0,1/2,0) 3/4,4/1,4 | (22) 2' x+1/2,0,1/2 |
| (25) 1' 1/2,1/2,1/2 | (26) b' (0,1/2,0) x,y,0 | (27) a' (1/2,0,0) x,0,z | (28) c' (0,0,1/2) z,y,0 |
| (29) 3' (1/2,1/2,1/2) x,x,z | (30) 3' x-1/2,x,x; | (31) 3' x-1/2,x,x+1/2,x; | (32) 3' x,x-1/2,x |
| (33) 3' (1/2,1/2,1/2) x,x,z | (34) 3' x+1/2,x-1/2,x; | (35) 3' x,x+1/2,x; | (36) 3' x,x+1/2,x |
| (37) 4' (0,1/2,0) 1/4,1/4,1/4 | (38) d (3/4,3/4,3/4) x,x,z | (39) 4' 0,1/4,z; 0,1/4,3/8 | (40) 4' 1/2,1/4,z; 1/2,1/4,1/4 |
| (41) 4' (0,1/2,0) 3/4,0,1/4 | (42) d (1/4,1/4,1/4) x,y+1/2,y | (43) d (3/4,3/4,3/4) x,y,y | (44) 4' x,1/2,1/4; 1/8,1/2,1/4 |
| (45) 4' (0,1/2,0) 1/4,1/4,1/4 | (46) d (1/4,1/4,1/4) x+1/2,x,y,x | (47) 4' 1/4,4,0; 1/4,3/8,0 | (48) d (3/4,3/4,3/4) x,y,x |

230.3.1649 - 3 - 3914
Continued 230.3.1649 la'^3'd

230.3.1649 - 4 - 3915

(29) \( \overline{z}, x, y \ [w, u, v] \)
(30) \( \overline{z} + 1/2, x + 1/2, y [w, u, v] \)
(31) \( z + 1/2, x, y + 1/2 [w, u, v] \)
(32) \( z, x + 1/2, y + 1/2 [w, u, v] \)

(33) \( \overline{y}, z, x \ [v, w, u] \)
(34) \( y, z + 1/2, x + 1/2 [v, w, u] \)
(35) \( y + 1/2, z + 1/2, x [v, w, u] \)
(36) \( y + 1/2, z, x + 1/2 [v, w, u] \)

(37) \( y + 1/4, x + 3/4, z + 3/4 [v, u, w] \)
(38) \( y + 1/4, x + 1/4, z + 1/4 [v, u, w] \)
(39) \( y + 3/4, x + 3/4, z + 1/4 [v, u, w] \)
(40) \( y + 3/4, x + 1/4, z + 3/4 [v, u, w] \)
(41) \( x + 1/4, z + 3/4, y + 3/4 [u, w, v] \)
(42) \( x + 3/4, z + 1/4, y + 3/4 [u, w, v] \)
(43) \( x + 1/4, z + 1/4, y + 1/4 [u, w, v] \)
(44) \( x + 3/4, z + 3/4, y + 1/4 [u, w, v] \)

(45) \( z + 1/4, y + 3/4, x + 1/4 [w, v, u] \)

48 g ..2'

1/8, y + 1/4 [u, v, v] \( 3/8, y, y + 3/4 [u, v, v] \)
(7/8, y + 1/4, 1/8, y [v, u, v] \( y + 1/4, 3/8, y [v, u, v] \)

(46) \( y + 3/4, 7/8, y [v, u, v] \)

ye + 3/4, 7/8, y [v, u, v] \( y + 1/4, 5/8, y [v, u, v] \)

y, y + 3/4, 7/8 [v, u, v] \( y, y + 1/4, 5/8 [v, u, v] \)

48 f 2.. x, 0, 1/4 [u, 0, 0] \( x + 1/2, 0, 3/4 [u, 0, 0] \)

0, 1/4, x [0, 0, u] \( 3/4, x + 1/2 [0, 0, u] \)

(47) x + 3/4, 1/2, 1/4 [u, 0, 0] \( x + 1/4, 0, 1/4 [u, 0, 0] \)

0, 3/4, x [0, u, 0] \( 1/4, x + 1/2 [0, u, 0] \)

(48) \( x + 1/4, 1/2, 3/4 [u, 0, 0] \)

32 e ..3.

x, x, x [u, u, u] \( x + 1/2, x, x + 1/2 [u, u, u] \)

x + 3/4, x + 1/4, z + 1/4 [u, u, u] \( x + 3/4, x + 3/4, x + 3/4 [u, u, u] \)

x, x, x [u, u, u] \( x + 1/2, x, x + 1/2 [u, u, u] \)

x + 1/2, x + 3/4, x + 3/4 [u, u, u] \( x + 1/2, x + 3/4, x + 3/4 [u, u, u] \)

12 d 4.. 3/8, 0, 1/4 [u, 0, 0] \( 1/8, 0, 3/4 [u, 0, 0] \)

0, 1/4, 3/8 [0, 0, u] \( 3/4, 1/8 [0, 0, u] \)

1/8, 1/2, 1/4 [u, 0, 0] \( 1/8, 0, 1/4 [u, 0, 0] \)

24 c 2.2' 1/8, 0, 1/4 [u, 0, 0] \( 7/8, 0, 3/4 [u, 0, 0] \)

0, 1/4, 1/8 [0, 0, u] \( 7/8, 0, 3/4 [u, 0, 0] \)

3/4, 7/8, 0 [0, u, 0] \( 0, 1/4, 5/8 [0, u, 0] \)
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>b</td>
<td>0.32'</td>
<td>1/8,1/8,1/8 [u,u,u]</td>
</tr>
<tr>
<td>16</td>
<td>a</td>
<td>0.3'</td>
<td>0,0,0 [0,0,0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3/4,1/4,1/4 [0,0,0]</td>
</tr>
</tbody>
</table>

**Symmetry of Special Projections**

Along [0,0,1] p4'm'm
- \(a^* = a/2\)
- \(b^* = b/2\)
- Origin at \(1/4,0,0\)

Along [1,1,1] p6mm
- \(a^* = (2a - b - c)/3\)
- \(b^* = (-a + 2b - c)/3\)
- Origin at \(x,x,x\)

Along [1,1,0] c\(_p\) 2'm'm'
- \(a^* = c/2\)
- \(b^* = -(a + b)/2\)
- Origin at \(x,x+1/4,1/8\)
### Symmetry Operations

**Origin** at center $(1/2,1/2,1/2)$

**Asymmetric unit**

- $1/8 < x < 1/8; -1/8 < y < 1/8; 0 < z < 1/4; max(x,-x,y,-y) < z$

**Vertices**

- $0,0,0$
- $1/8,1/8,1/8$
- $-1/8,1/8,1/8$
- $-1/8,-1/8,1/8$
- $1/8,-1/8,1/8$
- $1/8,1/8,1/4$
- $-1/8,1/8,1/4$
- $-1/8,-1/8,1/4$
- $1/8,-1/8,1/4$

**Symmetry Operations**

For $(0,0,0) + set$

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1</td>
<td>$(1,0,0,0)$</td>
<td>$(1/2,0,1/2)$</td>
</tr>
<tr>
<td>(2) 2</td>
<td>$(0,0,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(3) 3</td>
<td>$(0,1/2,0)$</td>
<td>$y,1/4$</td>
</tr>
<tr>
<td>(4) 4</td>
<td>$(1/2,0,0)$</td>
<td>$x,1/4,0$</td>
</tr>
<tr>
<td>(5) 3' x,x,x</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$x+1/2,x,x$</td>
</tr>
<tr>
<td>(6) 3' x,x,x</td>
<td>$(0,0,0,0)$</td>
<td>$1/2,1/2,0$</td>
</tr>
<tr>
<td>(7) 3' x,x,x</td>
<td>$(0,1/2,0,0)$</td>
<td>$y+1/2,0,1/2$</td>
</tr>
<tr>
<td>(8) 3' x,x,x</td>
<td>$(0,1/2,0,0)$</td>
<td>$y+1/2,0,1/2$</td>
</tr>
<tr>
<td>(9) 3' x,x,x</td>
<td>$(0,1/2,0,0)$</td>
<td>$y+1/2,0,1/2$</td>
</tr>
<tr>
<td>(10) 3' x,x,x</td>
<td>$(0,1/2,0,0)$</td>
<td>$y+1/2,0,1/2$</td>
</tr>
<tr>
<td>(11) 3' x,x,x</td>
<td>$(0,1/2,0,0)$</td>
<td>$y+1/2,0,1/2$</td>
</tr>
<tr>
<td>(12) 3' x,x,x</td>
<td>$(0,1/2,0,0)$</td>
<td>$y+1/2,0,1/2$</td>
</tr>
<tr>
<td>(13) 2' $x,x$</td>
<td>$(1/2,1/2,0)$</td>
<td>$x+1/2,1/2$</td>
</tr>
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<td>(14) 2' $x,x$</td>
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<td>(15) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
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<tr>
<td>(16) 4' $x$</td>
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</tr>
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<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(18) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(19) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(20) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(21) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(22) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(23) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(24) 4' $x$</td>
<td>$(0,0,0)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(25) 1</td>
<td>$(1/2,0,0)$</td>
<td>$x,y,1/4$</td>
</tr>
<tr>
<td>(26) 1</td>
<td>$(1/2,0,0)$</td>
<td>$x,y,1/4$</td>
</tr>
<tr>
<td>(27) 1</td>
<td>$(1/2,0,0)$</td>
<td>$x,y,1/4$</td>
</tr>
<tr>
<td>(28) 1</td>
<td>$(1/2,0,0)$</td>
<td>$x,y,1/4$</td>
</tr>
<tr>
<td>(29) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(30) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(31) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(32) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(33) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(34) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(35) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(36) 3' x,x,x</td>
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<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(37) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(38) 3' x,x,x</td>
<td>$(0,0,0)$</td>
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</tr>
<tr>
<td>(39) 3' x,x,x</td>
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</tr>
<tr>
<td>(40) 3' x,x,x</td>
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<tr>
<td>(41) 3' x,x,x</td>
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<tr>
<td>(42) 3' x,x,x</td>
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<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(43) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(44) 3' x,x,x</td>
<td>$(0,0,0)$</td>
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</tr>
<tr>
<td>(45) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(46) 3' x,x,x</td>
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<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(47) 3' x,x,x</td>
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<td>$1/2,1/2$</td>
</tr>
<tr>
<td>(48) 3' x,x,x</td>
<td>$(0,0,0)$</td>
<td>$1/2,1/2$</td>
</tr>
</tbody>
</table>

For $(1/2,1/2,1/2) + set$

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) t $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(2) t $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(3) t $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(4) t $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(5) 3 $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(6) 3 $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(7) 3 $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
<tr>
<td>(8) 3 $(1/2,1/2,1/2)$</td>
<td>$(1/2,1/2,1/2)$</td>
<td>$1/4,0,z$</td>
</tr>
</tbody>
</table>

230.4.1650 - 2 - 3918
Continued

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

Positions

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Coordinates</th>
</tr>
</thead>
</table>

96 | (0,0,0) + (1/2,1/2,1/2) + |

1  | x,y,z [u,v,w] |

230.4.1650 - 3 - 3919
Continued 230.4.1650

(29) \( z, x, y \ [w, u, v] \)

(30) \( z+1/2, x+1/2, y \ [w, u, v] \)

(31) \( z+1/2, x, y+1/2 \ [w, u, v] \)

(32) \( z, x+1/2, y+1/2 \ [w, u, v] \)

(33) \( y, z, x \ [v, w, u] \)

(34) \( y, z+1/2, x+1/2 \ [v, w, u] \)

(35) \( y+1/2, z+1/2, x \ [v, w, u] \)

(36) \( y+1/2, z, x+1/2 \ [v, w, u] \)

(37) \( y+1/4, x+3/4, z+3/4 \ [v, u, w] \)

(38) \( y+1/4, x+1/4, z+1/4 \ [v, u, w] \)

(39) \( y+3/4, x+3/4, z+1/4 \ [v, u, w] \)

(40) \( y+3/4, x+1/4, z+3/4 \ [v, u, w] \)

(41) \( x+1/4, z+3/4, y+3/4 \ [u, w, v] \)

(42) \( x+3/4, z+1/4, y+3/4 \ [u, w, v] \)

(43) \( x+1/4, z+1/4, y+1/4 \ [u, w, v] \)

(44) \( x+3/4, z+3/4, y+1/4 \ [u, w, v] \)

(45) \( z+1/4, y+3/4, x+3/4 \ [w, v, u] \)

48 g .2'

1/8, y, y+1/4 [u, v, v]

3/8, y+3/4 [u, v, v]

7/8, y+1/2, y+1/4 [v, u, v]

5/8, y+1/2, y+3/4 [u, u, v]

y+1/4,1/8, y [v, u, v]

y+3/4,3/8, y [v, u, v]

y+1/4,1/4,8, y [v, v, u]

y+1/4, y+3/4,3/8 [v, v, u]

7/8, y, y+3/4 [u, v, v]

5/8, y, y+1/4 [u, v, v]

y+3/4, 7/8, y [v, u, v]

y+1/4, 5/8, y [v, u, v]

y+1/4, 5/8, y+1/2 [v, v, u]

y+1/4, 3/8, y+1/2 [v, u, v]

y+1/2, y+3/4, 1/8 [v, v, u]

y+1/2, y+1/4, 3/8 [v, v, u]

48 f 2..

x, 0, 1/4 [u, 0, 0]

x+1/2, 0, 3/4 [u, 0, 0]

1/4, x, 0 [u, 0, 0]

3/4, x+1/2, 0 [u, 0, 0]

0, 1/4, x [0, 0, u]

0, 3/4, x+1/2 [0, 0, u]

3/4, x+1/4, 0 [u, 0, 0]

3/4, x+3/4, 1/2 [0, u, 0]

x+3/4, 1/2, 1/4 [u, 0, 0]

x+1/4, 0, 1/4 [u, 0, 0]

0, 1/4, x+1/4 [0, u, 0]

1/2, 1/4, x+3/4 [0, 0, u]

x+1/4, 0, 3/4 [u, 0, 0]

x+1/2, 0, 1/4 [u, 0, 0]

3/4, x+3/4, 0 [u, 0, 0]

1/4, x+1/4, 1/2 [0, u, 0]

0, 3/4, x [0, 0, u]

0, 1/4, x+1/2 [0, 0, u]

1/4, x+3/4, 0 [0, 0, u]

1/4, x+1/4, 1/2 [0, u, 0]

x+1/4, 1/2, 3/4 [u, 0, 0]

x+3/4, 0, 3/4 [u, 0, 0]

0, 3/4, x+3/4 [0, 0, u]

1/2, 3/4, x+1/4 [0, 0, u]

32 e .3.

x, x, x [u, u, u]

x+1/2, x, x+1/2 [u, u, u]

x, x+1/2, x+1/2 [u, u, u]

x+1/2, x+1/2, x [u, u, u]

x+3/4, x+1/4, x+1/4 [u, u, u]

x+3/4, x+3/4, x+3/4 [u, u, u]

x+1/4, x+1/4, x+1/4 [u, u, u]

x+1/4, x+3/4, x+1/4 [u, u, u]

x+1/4, x+1/4, x+1/4 [u, u, u]

x+3/4, x+1/4, x+3/4 [u, u, u]

12 d 4'.

3/8, 0, 1/4 [0, 0, 0]

1/8, 0, 3/4 [0, 0, 0]

1/4, 3/4, 8 [0, 0, 0]

3/4, 1/8, 0 [0, 0, 0]

0, 1/4, 3/8 [0, 0, 0]

0, 3/4, 1/8 [0, 0, 0]

3/4, 5/8, 0 [0, 0, 0]

3/4, 3/8, 1/2 [0, 0, 0]

1/8, 1/2, 1/4 [0, 0, 0]

7/8, 0, 1/4 [0, 0, 0]

0, 1/4, 7/8 [0, 0, 0]

1/2, 1/4, 1/8 [0, 0, u]

24 c 2.2'.

1/8, 0, 1/4 [u, 0, 0]

3/8, 0, 3/4 [u, 0, 0]

1/4, 1/8, 0 [u, 0, 0]

3/4, 3/8, 0 [u, 0, 0]

0, 1/4, 1/8 [0, 0, u]

0, 3/4, 3/8 [0, 0, u]

7/8, 0, 3/4 [u, 0, 0]

5/8, 0, 1/4 [u, 0, 0]

3/4, 7/8, 0 [u, 0, u]

1/4, 5/8, 0 [u, 0, u]

0, 3/4, 7/8 [0, 0, u]

0, 1/4, 5/8 [0, 0, u]

1/2, 3/4, 1/4 [0, 0, u]
| 16 | a | .3 | 0,0,0 [u,u,u] | 1/2,0,1/2 [u,u,u] | 0,1/2,1/2 [u,u,u] | 1/2,1/2,0 [u,u,u] |

**Symmetry of Special Projections**

Along [0,0,1]  \( p_2 \cdot 4mm \)
- \( a^* = a/2 \)
- \( b^* = b/2 \)
- Origin at 1/2,1/4,z

Along [1,1,1]  \( p_6'mm' \)
- \( a^* = (2a - b - c)/3 \)
- \( b^* = (-a + 2b - c)/3 \)
- Origin at x,x,x

Along [1,1,0]  \( c2'mm' \)
- \( a^* = c/2 \)
- \( b^* = -(a + b)/2 \)
- Origin at x,x+1/4,1/8
Origin at center \((\overline{3}')\)

Asymmetric unit \(-1/8 \leq x \leq 1/8;\ -1/8 \leq y \leq 1/8;\ 0 \leq z \leq 1/4;\ \max(x,-x,y,-y) \leq z\)

Vertices
\[
\begin{aligned}
0,0,0 & \\
1/8,1/8,1/8 & \\
-1/8,1/8,1/8 & \\
1/8,1/8,1/4 & \\
-1/8,1/8,1/4 & \\
1/8,1/8,1/4 & \\
1/8,1/8,1/4 & \\
-1/8,-1/8,1/8 & \\
1/8,-1/8,1/8 & \\
-1/8,-1/8,1/4 & \\
1/8,-1/8,1/4 & \\
\end{aligned}
\]

Symmetry Operations

For \((0,0,0)\) + set

\[
\begin{array}{lllll}
(1) 1 & (2) 2 (0,0,1/2) 1/4,0,z & (3) 2 (0,1/2,0) 0,y,1/4 & (4) 2 (1/2,0,0) x,1/4,0 \\
(1,0,0,0) & (2_2 1/2,0,1/2) & (2_2 0,1/2,1/2) & (2_2 1/2,1/2,0) & \\

(5) 3' \ x,\ x,\ x & (6) 3' \ x+1/2,\ x,\ x & (7) 3' \ x+1/2,\ x-1/2,\ x & (8) 3' \ x,\ x+1/2,\ x \\
(3_{xyz} 0,0,0) & (3_{xyz} 1/2,1/2,0) & (3_{xyz} 1/2,0,1/2) & (3_{xyz} 0,1/2,1/2) & \\

(9) 3' \ x,\ x,\ x & (10) 3' \ (-1/3,1/3,1/3) \ x+1/6,\ x+1/6,\ x & (11) 3' \ (1/3,1/3,-1/3) \ x+1/3,\ x+1/6,\ x & (12) 3' \ (1/3,-1/3,1/3) \ x-1/6,\ x+1/3,\ x & \\
(3_{xyz} 0,0,0) & (3_{xyz} 1/2,1/2,0) & (3_{xyz} 1/2,0,1/2) & (3_{xyz} 1/2,0,1/2) & \\

(13) 2 (1/2,1/2,0) x,x-1/4,1/8 & (14) 2 (0,1/2,1/2) x,x+3/4,3/8 & (15) 4' \ (0,3/4,0) 1/4,0,z & (16) 4' \ (0,1/4,1/2) 1/4,1/4,1/4 & \\
(2_{xy} 3/4,1/4,1/4) & (2_{xy} 3/4,3/4,1/4) & (4_{z} 3/4,3/4,1/4) & (4_{z} 3/4,3/4,1/4) & \\

(17) 4' \ (3/4,0,0) x,1/4,0 & (18) 2 (0,1/2,1/2) 1/8,y+1/4,y & (19) 2 (0,3/4,1/4) y-3/4,\ y & (20) 4' \ (1/4,0,0) x,-1/4,1/2 & \\
(4_{z} 3/4,1/4,1/4) & (2_{xy} 1/4,1/4,1/4) & (2_{xy} 3/4,3/4,1/4) & (4_{z} 1/4,1/4,3/4) & \\

(21) 4' \ (0,1/4,0) 1/2,y,-1/4 & (22) 2 (1/2,0,1/2) x-1/4,1/8,x & (23) 4' \ (0,3/4,0) 0,y,1/4 & (24) 2 \ x+3/4,3/8,x & \\
(4_{z} 3/4,1/4,1/4) & (2_{xy} 1/4,1/4,1/4) & (4_{z} 3/4,3/4,1/4) & (2_{xy} 3/4,3/4,1/4) & \\

(25) \ 1' \ 0,0,0 & (26) a' \ (1/2,0,0) y,0,1/4 & (27) c' \ (0,0,1/2) x,1/4,z & (28) b' \ (0,1/2,0) 1/4,y,z & \\
(1 0,0,0)' & (m_{xy} 1/2,0,1/2)' & (m_{y} 0,1/2,1/2)' & (m_{y} 0,1/2,1/2)' & \\

(29) 3' \ x,x; 0,0,0 & (30) 3' \ x-1/2,x+1,x; 0,1/2,1/2 & (31) 3' \ x+1/2,x+1/2,x; 1/2,1/2,0 & (32) 3' \ x+1/2,x+1/2,x; 2,1/2,0 & \\
(3_{xyz} 0,0,0)' & (3_{xyz} 1/2,1/2,0)' & (3_{xyz} 1/2,0,1/2)' & (3_{xyz} 1/2,0,1/2)' & \\

(33) 3' \ x,x; 0,0,0 & (34) 3' \ x+1/2,x-1/2,x; 0,0,1/2 & (35) 3' \ x,x+1/2,x; 0,1/2,0 & (36) 3' \ x+1/2,x+1/2,x; 1/2,0,0 & \\
(3_{xyz} 0,0,0)' & (3_{xyz} 0,1/2,1/2)' & (3_{xyz} 1/2,1/2,0)' & (3_{xyz} 1/2,0,1/2)' & \\

(37) d' \ (-1/4,1/4,1/4) x+1/2,\ x,z & (38) d' \ (1/4,1/4,1/4) x,x,z & (39) 4' \ x,x; 0,3/4,1/4; 0,3/4,1/4 & (40) 4' \ x,-1/4,z; 1/2,-1/4,1/2 & \\
(m_{x} 1/4,3/4,3/4)' & (m_{xy} 1/4,1/4,1/4)' & (4_{z} 3/4,3/4,1/4)' & (4_{z} 3/4,1/4,3/4)' & \\

(41) 4' \ x,0,3/4; 1/8,0,3/4 & (42) d' \ (3/4,1/4,1/4) x,y+1/2,\ y & (43) 4' \ x,0,3/4; 1/8,0,3/4 & (44) 4' \ x,1/2,-1/4; 3/8,1/2,-1/4 & \\
(4_{z} 1/4,3/4,1/4)' & (m_{xy} 3/4,1/4,1/4)' & (m_{xy} 1/4,1/4,1/4)' & (4_{z} 3/4,1/4,3/4)' & \\

(45) 4' \ x,-1/4,y,1/2; -1/4,3/8,1/2; 46' d' \ (1/4,3/4,1/4) x+y+1/2,\ y & (47) 4' \ x,-1/4,y,1/2; -1/4,3/8,1/2; 46' d' \ (1/4,3/4,1/4) x,y+1/2,\ y & (48) 4' \ x,-1/4,y,1/2; -1/4,3/8,1/2; 46' d' \ (1/4,3/4,1/4) x,y+1/2,\ y & (48) 4' \ x,-1/4,y,1/2; -1/4,3/8,1/2; 46' d' \ (1/4,3/4,1/4) x,y+1/2,\ y & \\
(4_{y} 1/4,3/4,1/4)' & (m_{xz} 3/4,3/4,1/4)' & (m_{xz} 1/4,1/4,1/4)' & (m_{xz} 1/4,1/4,1/4)' & \\

For \((1/2,1/2,1/2)\) + set

\[
\begin{array}{llll}
(1) t (1/2,1/2,1/2) & (2) 2 0,1/4,z & (3) 2 1/4,y,0 & (4) 2 x,0,1/4 \\
(1 1/2,1/2,1/2) & (2_2 0,1/2,0) & (2_2 1/2,0,0) & (2_2 0,0,1/2) & \\

(5) 3' \ (1/2,1/2,1/2) x,x,x & (6) 3' \ (1/6,-1/6,1/6) x-1/6,x+1/3,\ x & (7) 3' \ (-1/6,1/6,1/6) x+1/6,x+1/6,\ x & (8) 3' \ (1/6,1/6,-1/6) x+1/3,\ x+1/6,\ x & \\
(3_{xyz} 1/2,1/2,1/2) & (3_{xyz} 1/2,1/2,1/2) & (3_{xyz} 1/2,1/2,1/2) & (3_{xyz} 1/2,1/2,1/2) & \\
\end{array}
\]
Continued

(9) 3' (1/2,1/2,1/2) x,x,x
(10) 3' (1/6, -1/6, -1/6) x+1/6, x+1/6, x
(3,xyz) 1/2,1/2,1/2

(11) 3' (-1/6, 1/6, 1/6) x+1/3, x+1/3, x
(3,xyz) 1/2,1/2,1/2

(12) 3' (-1/6, 1/6, -1/6) x+1/6, x+1/6, x
(3,xyz) 1/2,1/2,1/2

(13) 2 (1/2,1/2,0) x,x+1/4,3/8
(2,xyz) 1/4,3/4,3/4

(14) 2 x,x+1/4,1/8
(2,xyz) 1/4,1/4,1/4

(15) 4' (0,0,1/4) 3/4,0,z
(4,-1) 3/4,3/4,1/4

(16) 4' (0,0,3/4) 1/4,1/2,z
(4,-1) 3/4,3/4,1/4

(17) 4' (1/4,0,0) x,3/4,0
(4,-1) 1/4,3/4,3/4

(18) 2 (0,1/2,1/2) 3/8,y-1/4,y
(2,xyz) 1/4,1/4,1/4

(19) 2 1/8,y+1/4,y
(2,xyz) 1/4,1/4,1/4

(20) 4' (3/4,0,0) x,1/4,1/2
(4,-1) 3/4,3/4,1/4

(21) 4' (0,3/4,0) 1/2,y,1/4
(4,-1) 1/4,3/4,3/4

(22) 2 (1/2,0,1/2) x+1/4,3/8,x
(2,xyz) 3/4,3/4,1/4

(23) 4' (0,1/2,0) 0,y,3/4
(4,-1) 3/4,1/4,1/4

(24) 2 1/2,1/4,1/8,x
(2,xyz) 1/4,1/4,1/4

(25) 'd' 1/4,1/4,1/4
(1,1,1/2,1/2)

(26) b' (0,1/2,0) x,y,0
(m,0,1/2,0)

(27) a' (1/2,0,0) x,0,z
(m,1/2,0,0)

(28) c' (0,0,1/2) y,z,0
(m,0,0,1/2)

(29) 3' x,x,x;
(3,xyz) 1/2,1/2,1/2

(30) 3' x-1/2,x,x;
(3,xyz) 1/2,1/2,1/2

(31) 3' x-1/2,x,x+1/2,x;
(3,xyz) 1/2,1/2,1/2

(32) 3' x,x-1/2,x;
(3,xyz) 1/2,1/2,1/2

(33) 3' x,x,x;
(3,xyz) 1/2,1/2,1/2

(34) 3' x+1/2,x-1/2,x;
(3,xyz) 1/2,1/2,1/2

(35) 3' x,x+1/2,x;
(3,xyz) 1/2,1/2,1/2

(36) 3' x+1/2,x,x;
(3,xyz) 1/2,1/2,1/2

(37) d' (1/4,1/4,1/4) x+1/2,x,z
(3,xyz) 3/4,3/4,3/4

(38) d' (3/4,3/4,3/4) x,x,z
(m,0,1/2,0)

(39) d' 0,1/4,z; 0,1/4,3/8
(4,-1) 1/4,1/4,1/4

(40) d' 1/2,1/4,z; 1/2,1/4,1/4
(4,-1) 1/4,3/4,1/4

(41) d' x,0,1/4; 3/8,0,1/4
(4,-1) 3/4,1/4,1/4

(42) d' (1/4,1/4,1/4) x,y+1/2,y
(4,-1) 3/4,3/4,3/4

(43) d' (3/4,3/4,3/4) x,y,y
(m,0,1/2,0)

(44) d' x,1/2,1/4; 1/8,1,2,1/4
(4,-1) 1/4,1,4,3/4

(45) d' (1/4,1/4,1/4) x+1/2,y,x
(4,-1) 3/4,1/4,1/4

(46) d' (1/4,1/4,1/4) x+1/2,y,x
(4,-1) 1/4,1/4,1/4

(47) d' 1/4,y,0; 1/4,3/8,0
(4,-1) 1/4,3/4,1/4

(48) d' (3/4,3/4,3/4) x,y,x
(m,0,1/2,0)

Generators selected

(1); t(1,0,0); t(0,1,0); t(0,0,1); t(1/2,1/2,1/2); (2); (3); (5); (13); (25).

Positions

Multiplicity, Wyckoff letter, Site Symmetry.

96  h  1

(1) x,y,z [u,v,w]
(2) x+1/2,y,z+1/2 [u,v,w]
(3) x,y+1/2,z+1/2 [u,v,w]
(4) x+1/2,y+1/2,z [u,v,w]

(5) z,x,y [w,u,v]
(6) z+1/2,x+1/2,y [w,u,v]
(7) z+1/2,x,y+1/2 [w,u,v]
(8) z,x+1/2,y+1/2 [w,u,v]

(9) y,z,x [v,w,u]
(10) y,z+1/2,x+1/2 [v,w,u]
(11) y+1/2,z+1/2,x [v,w,u]
(12) y+1/2,z+1/2 [v,w,u]

(13) y+3/4,x+1/4,z+1/4 [v,u,w]
(14) y+3/4,x+3/4,z+3/4 [v,u,w]
(15) y+1/4,x+1/4,z+3/4 [v,u,w]
(16) y+1/4,x+3/4,z+1/4 [v,u,w]
(17) x+3/4,z+1/4,y+1/4 [u,w,v]
(18) x+1/4,z+3/4,y+1/4 [u,w,v]
(19) x+3/4,z+3/4,y+1/4 [u,w,v]
(20) x+1/4,z+1/4,y+3/4 [u,w,v]
(21) z+3/4,y+1/4,x+1/4 [w,v,u]
(22) z+1/4,y+3/4,x+1/4 [w,v,u]
(23) z+1/4,y+3/4,x+3/4 [w,v,u]
(24) z+3/4,y+3/4,x+3/4 [w,v,u]
(25) x,y,z [u,v,w]
(26) x+1/2,y+1/2 [u,v,w]
(27) x,y+1/2,z+1/2 [u,v,w]
(28) x+1/2,y+1/2,z [u,v,w]
Symmetry of Special Projections

<table>
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<th>16 b</th>
<th>.32</th>
<th>1/8,1/8,1/8 [0,0,0]</th>
<th>3/8,7/8,5/8 [0,0,0]</th>
<th>7/8,5/8,3/8 [0,0,0]</th>
<th>5/8,3/8,7/8 [0,0,0]</th>
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<tr>
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<td>.3'</td>
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<td>1/2,1/2,0 [0,0,0]</td>
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<td>3/4,3/4,3/4 [0,0,0]</td>
<td>1/4,1/4,3/4 [0,0,0]</td>
<td>1/4,3/4,1/4 [0,0,0]</td>
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