



Complete online database of maximal subgroups of subperiodic groups at the Bilbao Crystallographic Server

Gemma de la Flor,^{a*} Hans Wondratschek^{b‡} and Mois I. Aroyo^c

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‡ Deceased.

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The section of the Bilbao Crystallographic Server (<https://www.cryst.ehu.es>) dedicated to subperiodic groups includes the program *MAXSUB*, which gives online access to the complete database of maximal subgroups of subperiodic groups. All maximal non-isotypic subgroups as well as all maximal isotypic subgroups of indices up to 9 are listed individually, together with the series of maximal isotypic subgroups of subperiodic groups. These data were compared with those of Litvin [(2013), *Magnetic group tables, 1-, 2- and 3-dimensional subperiodic groups and magnetic space groups*], which revealed several differences, discussed here in detail.

1. Introduction

Crystallographic information about space groups is published in *International tables for crystallography*, Vol. A, *Space-group symmetry* (Aroyo, 2016; henceforth abbreviated as *ITA*). The complete listing of the maximal subgroups of all 230 space groups, however, is available in *International tables for crystallography*, Vol. A1, *Symmetry relations between space groups* (Wondratschek & Müller, 2010; henceforth abbreviated as *ITA1*). Aside from the subgroups of space groups with three-dimensional lattices which are again space groups, there also exist subgroups called subperiodic groups with translation lattices of dimensions one or two. These are the groups required to describe polymers, nanotubes, nanowires and layered materials (Müller, 2017; Gorelik *et al.*, 2021; de la Flor & Milošević, 2024).

The interest in materials with subperiodic symmetry is constantly growing due to their outstanding properties and possible technological applications (Xu *et al.*, 2013). There are three types of subperiodic groups: *frieze groups* (two-dimensional groups with one-dimensional translation lattices), *rod groups* (three-dimensional groups with one-dimensional translation lattices) and *layer groups* (three-dimensional groups with two-dimensional translation lattices). Frieze groups do not correspond to any physical atomic structure, as real objects cannot be strictly confined to a two-dimensional space. While they are useful for describing physical properties and geometric patterns, they have no direct application to real structures. The crystallographic data for subperiodic groups are compiled in *International tables for crystallography*, Vol. E, *Subperiodic groups* (Kopský & Litvin, 2010; henceforth referred to as *ITE*). Since there is not a volume in *International tables for crystallography* for subperiodic groups similar to *ITA1*, the maximal subgroups of subperiodic groups are

Maximal Subgroups of Rod Group $p2_12$ (No. 64)

Note: The program uses the default settings.

In the following table the list of maximal subgroup types is given. Click over "show." to see the complete list of subgroups and their distribution in classes of conjugate subgroups.

N	Subgroup	HM	Symbol	Index	Type	Transformations
1	13	$p2_12$	3	1	show.	
2	48	$p3_112$	2	1	show.	
3	55	$p6_1$	2	1	show.	
4	63	$p6_22$	2	k	show.	
5	64	$p6_22$	7	k	show.	
6	66	$p6_22$	2	k	show.	
7	66	$p6_22$	5	k	show.	

[Click here to see the Series of Maximal Subgroups]

1 represents the translationengleichen subgroups
k represents the klassengleichen subgroups

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listed in *ITE*. This listing follows the format of *ITA* (Hahn, 2002) but lacks additional information, such as a complete list of maximal subgroups. It also omits the series of maximal isotypic subgroups of subperiodic groups, where isotypic refers to subgroups belonging to the same *subperiodic group type*. (One often refers to the layer, rod and frieze groups without distinguishing between the terms layer group type, rod group type and frieze group type. In many cases, this distinction is not necessary, and in order to avoid unnecessarily lengthy terminology, the same approach is taken in this article.) Additionally, the minimal supergroups are not included in *ITE*. To the best of our knowledge, the only complete compilation of maximal subgroups of subperiodic groups, but only of indices up to 4, can be found in *Magnetic group tables, 1-, 2- and 3-dimensional subperiodic groups and magnetic space groups* (Litvin, 2013; henceforth referred to as Litvin's book), an electronic book of about 12000 pages. However, the series of maximal isotypic subgroups of subperiodic groups are also not available.

The complete data about the maximal subgroups of subperiodic groups are now available online in the databases of the Bilbao Crystallographic Server (<https://www.cryst.ehu.es>) (Aroyo *et al.*, 2011; Tasci *et al.*, 2012; hereafter referred to as BCS), in the section *Subperiodic groups: layer, rod and frieze groups*. In contrast to *ITE*, the BCS database of maximal subgroups of subperiodic groups provides the complete listing (not just by type but individually) of all maximal non-isotypic and all maximal isotypic subgroups of subperiodic groups of indices up to 9. The list of maximal subgroups is retrieved by the program *MAXSUB*, which also gives access to the series of maximal isotypic subgroups of subperiodic groups.

The aim of this contribution is to present the complete database of maximal subgroups and series of maximal isotypic subgroups of subperiodic groups available in the BCS. The procedure applied to derive the maximal subgroups of subperiodic groups is described in Section 3. The data from Litvin's book were reviewed and compared with those from the BCS, and their differences are listed in Section 5 in detail.

2. Subperiodic groups

Subperiodic groups are two- and three-dimensional groups with one- and two-dimensional translations. The 80 layer groups together with the 75 rod groups and the seven frieze groups constitute the subperiodic groups. The section *Subperiodic groups: layer, rod and frieze groups* of the BCS hosts the subperiodic groups crystallographic databases. The structure of these databases is similar to that of the space groups – they include information on generators, general positions, Wyckoff positions and maximal subgroups for subperiodic groups. Apart from the data shown in *ITE*, the server offers additional information and computer tools that allow the generation of data not available in *ITE*. The BCS also hosts the Brillouin-zone database for layer groups (de la Flor *et al.*, 2021) and more complex programs to calculate, for example, the site-symmetry induced representations of layer

groups (de la Flor *et al.*, 2019). Note that in the programs of the BCS the Hermann–Mauguin symbols for frieze and rod groups do not use the calligraphy font used in *ITE* to depict the Bravais-lattice type, *i.e.* the frieze group $\rho 2mg$ (No. 7) and the rod group ρmcm (No. 22) are represented as $p2mg$ and ρmcm in the BCS, respectively.

The programs and databases of the BCS related to subperiodic groups use the standard or default settings of the subperiodic groups. These are the specific settings of subperiodic groups that coincide with the conventional subperiodic group descriptions found in *ITE*. For layer groups with more than one description in *ITE*, the following settings are chosen as standard: (i) *cell-choice 1* description for the two monoclinic/oblique layer groups $p11a$ (No. 5) and $p112/a$ (No. 7) given with respect to three cell choices in *ITE*, and (ii) *origin choice 2* descriptions (*i.e.* when the origin is at a centre of inversion) for the three layer groups $p4/n$ (No. 52), $p4/nbm$ (No. 62) and $p4/nmm$ (No. 64) listed with respect to two origins in *ITE*. For rod groups, the first setting is chosen as standard for the trigonal and hexagonal groups with two descriptions (*cf.* Table 1.2.6.3 of *ITE*).

Following the conventions of *ITE*, the *ab* plane is the plane of periodicity for layer groups; this means that the translation vectors are of the form

$$\begin{pmatrix} t_1 \\ t_2 \\ 0 \end{pmatrix},$$

where t_1 and t_2 are integer numbers.

For rod groups, the *c* axis is the line of periodicity and the translation vectors are of the form

$$\begin{pmatrix} 0 \\ 0 \\ t_3 \end{pmatrix},$$

where t_3 is an integer number.

In the case of frieze groups, the periodicity is along the *a* axis; therefore, the translation vectors are of the form

$$\begin{pmatrix} t_1 \\ 0 \end{pmatrix}.$$

As in space groups, for subperiodic groups a group-subgroup pair $\mathcal{H} < \mathcal{S}$ is also characterized by the group \mathcal{S} , subgroup \mathcal{H} , index $[i]$ and transformation matrix-column pair (\mathbf{P}, \mathbf{p}) relating the basis of \mathcal{H} and \mathcal{S} . The matrix-column pair (\mathbf{P}, \mathbf{p}) describes a coordinate transformation and consists of two parts:

(i) A linear part \mathbf{P} , denoted by a (3×3) matrix for rod and layer groups and by a (2×2) matrix for frieze groups, describing the change of direction and/or length of the basis vectors:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}')_H = (\mathbf{a}, \mathbf{b}, \mathbf{c})_S \mathbf{P} \quad \text{for rod and layer groups,}$$

$$(\mathbf{a}', \mathbf{b}')_H = (\mathbf{a}, \mathbf{b})_S \mathbf{P} \quad \text{for frieze groups,}$$

where $(\mathbf{a}', \mathbf{b}', \mathbf{c}')_H$ and $(\mathbf{a}', \mathbf{b}')_H$ represent the bases of the subgroup \mathcal{H} and $(\mathbf{a}, \mathbf{b}, \mathbf{c})_S$ and $(\mathbf{a}, \mathbf{b})_S$ the bases of the subperiodic group \mathcal{S} .

(ii) An origin shift \mathbf{p} denoted by a (3×1) column vector $\mathbf{p} = (0, 0, p_3)$ for rod groups and $\mathbf{p} = (p_1, p_2, 0)$ for layer groups; and by a (2×1) column vector $\mathbf{p} = (p_1, 0)$ for frieze groups. The coefficients of \mathbf{p} describe the position of the origin $O_{\mathcal{H}}$ of \mathcal{H} referred to the coordinate system of \mathcal{S} .

The data of the matrix–column pair (\mathbf{P}, \mathbf{p}) are often written in the following concise form for rod and layer groups:

$$P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \\ P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}; p_1, p_2, p_3,$$

where $p_1 = p_2 = 0$ for rod groups and $p_3 = 0$ for layer groups. For frieze groups, the form is

$$P_{11}\mathbf{a} + P_{21}\mathbf{b}, P_{12}\mathbf{a} + P_{22}\mathbf{b}; p_1, 0.$$

3. Derivation of the maximal subgroups of subperiodic groups based on the group–subgroup relations between subperiodic and space groups

A group–subgroup relationship exists between subperiodic groups \mathcal{S} and space groups \mathcal{G} , i.e. $\mathcal{S} < \mathcal{G}$. For each subperiodic group, there is a two- or three-dimensional space group \mathcal{G} with the same symmetry diagram and general-position diagram. These relationships have been considered in detail in the literature [see e.g. Wood (1964), *ITE* and references therein]. The type of space group of which a given subperiodic group is a subgroup is not defined uniquely. The ‘simplest’ space group \mathcal{G} to which \mathcal{S} is related can be expressed as a semi-direct product of \mathcal{S} with a one- or two-dimensional translation group \mathcal{T}_i of additional translations $\mathcal{G} = \mathcal{T}_i \wedge \mathcal{S}$, where \mathcal{T}_i is a normal subgroup of \mathcal{G} (Evarestov & Smirnov, 1993; Smirnov & Tronc, 2006). Thus, subperiodic groups \mathcal{S} are isomorphic to factor groups $\mathcal{G}/\mathcal{T}_i$ (Litvin & Kopský, 1987, 2000). In the case of layer groups \mathcal{L} (defined as a three-dimensional crystallographic group with periodicity restricted to a two-dimensional subspace), the three-dimensional space group \mathcal{G} to which a layer group \mathcal{L} is related can be expressed as a semi-direct product of \mathcal{L} with the one-dimensional translation group \mathcal{T}_3 of additional translations $\mathcal{G} = \mathcal{T}_3 \wedge \mathcal{L}$. As a result of this, the layer group \mathcal{L} is isomorphic with the factor group $\mathcal{G}/\mathcal{T}_3$. For rod groups \mathcal{R} (defined as a three-dimensional crystallographic group with periodicity restricted to a one-dimensional subspace), the three-dimensional group \mathcal{G} to which a rod group \mathcal{R} is related can be represented as a semi-direct product of \mathcal{R} and the two-dimensional translation group \mathcal{T}_2 of additional translations $\mathcal{G} = \mathcal{T}_2 \wedge \mathcal{R}$. This means that the rod group \mathcal{R} is isomorphic with the factor group $\mathcal{G}/\mathcal{T}_2$. Finally, for frieze groups \mathcal{F} (defined as a two-dimensional crystallographic group with periodicity restricted to a two-dimensional subspace), the two-dimensional space group \mathcal{G} (plane group) to which a frieze group \mathcal{F} is related can be expressed as a semi-direct product of \mathcal{F} with the one-dimensional translation

Table 1

Maximal subgroups of indices up to 4 for the space group $P4$ (No. 75).

Subgroups marked with t are *translationengleiche* and those marked with k are *klassengleiche*.

Group	Index	Type	(\mathbf{P}, \mathbf{p})
$P112$ (No. 3, $P2$)	2	t	$\mathbf{b}, \mathbf{c}, \mathbf{a}$
$P4$ (No. 75)	2	k	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$ $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}; \frac{1}{2}, \frac{1}{2}, 0$
$P4$ (No. 75)	3	k	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$
$P4_2$ (No. 74)	2	k	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
$I4$ (No. 79)	2	k	$\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$ $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}; \frac{1}{2}, \frac{1}{2}, 0$

group \mathcal{T}_1 of additional translations $\mathcal{G} = \mathcal{T}_1 \wedge \mathcal{F}$. Therefore, the frieze group \mathcal{F} is isomorphic with the factor group $\mathcal{G}/\mathcal{T}_1$.

The isomorphism between the subperiodic group \mathcal{S} and the factor group $\mathcal{G}/\mathcal{T}_i$ results in a close relationship between the Wyckoff positions, maximal subgroups, minimal supergroups and irreducible representations of \mathcal{S} and \mathcal{G} . For example, one can show that the set of Wyckoff positions of a subperiodic group is contained in the set of Wyckoff positions of the related space (or plane) group (cf. Evarestov & Smirnov, 1993). The restrictions imposed by the loss of periodicity result in the restrictions of the special-position coordinates of subperiodic groups.

The maximal subgroups of subperiodic groups \mathcal{S} can be derived from the maximal subgroups of the two- or three-dimensional space groups, since the set of maximal subgroups of a subperiodic group is contained in the set of maximal subgroups of the related space group. The maximal subgroups database for subperiodic groups was constructed from the maximal subgroups database of two- and three-dimensional space groups provided by the BCS (Aroyo *et al.*, 2006). These subgroups were classified into two types: *translationengleiche* and *klassengleiche* subgroups (for further details, see Appendix A). Additionally, the classification of maximal subgroups of subperiodic groups into conjugacy classes can be derived from the corresponding classification for space groups. Consider the subgroups \mathcal{H}_i and \mathcal{H}_k , which are subgroups of the space group \mathcal{G} and the subperiodic group \mathcal{S} (where \mathcal{S} is isomorphic to the factor group $\mathcal{G}/\mathcal{T}_i$). These two subgroups, \mathcal{H}_i and \mathcal{H}_k , are said to be conjugate if there exists an element g of the space group \mathcal{G} such that $g\mathcal{H}_i g^{-1} = \mathcal{H}_k$. Furthermore, if g is an element of the subperiodic group \mathcal{S} , then \mathcal{H}_i and \mathcal{H}_k remain conjugate subgroups within \mathcal{S} as well. As an example, let us determine the maximal subgroups of indices up to 4 for the layer group $p4$ (No. 49) and the rod group $\mu 4$ (No. 23), isomorphic to factor groups $P4/\mathcal{T}_3$ and $P4/\mathcal{T}_2$, respectively. Table 1 shows the maximal subgroups of indices up to 4 for the space group $P4$ (No. 75). The loss of periodicity along the z direction restricts the maximal subgroups of layer groups: only the maximal subgroups of \mathcal{G} without loss of translations along the c axis are maximal subgroups of the layer groups. In this case, there are three maximal subgroups for the layer group $p4$: one *translationengleiche* subgroup $p112$ (No. 3) of index 2 and transformation matrix $(\mathbf{P}, \mathbf{p}) = \mathbf{a}, \mathbf{b}, \mathbf{c}$, and two

Table 2

Series of maximal isomorphic subgroups of the space group $P4$ (No. 75).

For each of the series, the Hermann–Mauguin symbol of the subgroup, the index, the transformation matrix (\mathbf{P}, \mathbf{p}) relating the group and the subgroup, and the restriction conditions on the parameters describing the series are provided.

	Subgroup	Index	(\mathbf{P}, \mathbf{p})	Conditions
Series #1	$P4$ (No. 49)	p	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & p & 0 \end{pmatrix}$	p prime
Series #2	$P4$ (No. 49)	p^2	$\begin{pmatrix} p & 0 & 0 & u \\ 0 & p & 0 & v \\ 0 & 0 & 1 & 0 \end{pmatrix}$	prime $p > 2$ $p = 4n - 1$ $0 \leq u < p$ $0 \leq v < p$
Series #3	$P4$ (No. 49)	$p = q^2 + r^2$	$\begin{pmatrix} q & r & 0 & u \\ -r & q & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	prime $p > 4$ $p = 4n + 1$ $q > 0; r > 0$ $0 \leq u < p$

klassengleiche subgroups $p4$ (No. 49) of index 2 and transformation matrices $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}$ and $\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}; \frac{1}{2}, \frac{1}{2}, 0$.

The loss of periodicity along the x and y directions restricts the maximal subgroups of rod groups: only the maximal subgroups of \mathcal{G} without loss of translations along the a and b axes are maximal subgroups of the rod groups. Therefore, for the rod group $\mu 4$ (No. 23) there are four maximal subgroups: (i) the *translationengleiche* subgroup $\mu 112$ (No. 8) of index 2 and $(\mathbf{P}, \mathbf{p}) = \mathbf{a}, \mathbf{b}, \mathbf{c}$; (ii) the *klassengleiche* subgroup $\mu 4$ (No. 23) of index 2 and $(\mathbf{P}, \mathbf{p}) = \mathbf{a}, \mathbf{b}, 2\mathbf{c}$; (iii) the *klassengleiche* subgroup $\mu 4$ (No. 23) of index 3 and $(\mathbf{P}, \mathbf{p}) = \mathbf{a}, \mathbf{b}, 3\mathbf{c}$; and (iv) the *klassengleiche* subgroup $\mu 4_2$ (No. 25) of index 2 and $(\mathbf{P}, \mathbf{p}) = \mathbf{a}, \mathbf{b}, 2\mathbf{c}$.

The rest of the maximal subgroups of subperiodic groups of indices up to 9 were calculated from the series of maximal isotypic subgroups of subperiodic groups. These series can also be directly derived from the series of maximal isomorphic subgroups of space groups. For example, for the space-group type $P4$ there are three series of maximal isomorphic subgroups (see Table 2). Two of these series, Series #2 and #3, are also the series of maximal isotypic subgroups for the layer group $p4$ since the loss of translations occurs in the ab plane. For the rod group $\mu 4$, however, only one series of maximal isotypic subgroups exists with loss of translations along the c axis; this corresponds to the Series #1 in Table 2.

4. The program MAXSUB

The database of the maximal subgroups of subperiodic groups of the BCS is accessible from the *MAXSUB* program (https://www.cryst.ehu.es/subperiodic/get_sub_maxsub.html) in the section *Subperiodic groups: layer, rod and frieze groups*. This provides the complete listing of (i) all maximal non-isotypic subgroups for each subperiodic group, and (ii) all maximal isotypic subgroups of indices up to 9. In addition to this, there is also an option in the program to retrieve the series of maximal isotypic subgroups.

The subperiodic-group type (frieze, rod or layer) and the corresponding *ITE* number of the group are required as input to the program *MAXSUB*. If the *ITE* number is unknown, this

can be selected from a table with the Hermann–Mauguin symbols of the selected subperiodic-group type. The program first returns a table with the maximal subgroup \mathcal{H} of the selected subperiodic group \mathcal{S} (see Fig. 1). Each subgroup $\mathcal{H} < \mathcal{S}$ is specified by its *ITE* number, Hermann–Mauguin symbol, index and subgroup type (t for *translationengleiche* or k for *klassengleiche* subgroup, see Appendix A and Section 2.2.4 of *ITA1*). The complete list of subgroups and their distribution in classes of conjugate subgroups is obtained by clicking on the link ‘show..’. For example, the rod group $\mu 6_2 22$ (No. 64) has two maximal *klassengleiche* subgroups $\mu 6_1 22$ (No. 63) of index 2 distributed in two conjugacy classes of conjugate subgroups (see Fig. 2). The transformation matrix–column pairs (\mathbf{P}, \mathbf{p}) that relate the standard basis of \mathcal{H} and \mathcal{S} are also provided by the program.

Maximal Subgroups of Rod Group $\mu 6_2 22$ (No. 64)

Note: The program uses the default settings

In the following table the list of maximal subgroup types is given. Click over ‘show..’ to see the complete list of subgroups and their distribution in classes of conjugate subgroups.

N	Subgroup	HM Symbol	Index	Type	Transformations
1	13	$\mu 2 2 2$	3	t	show..
2	48	$\mu 3_2 1 2$	2	t	show..
3	55	$\mu 6_2$	2	t	show..
4	63	$\mu 6_1 2 2$	2	k	show..
5	64	$\mu 6_2 2 2$	7	k	show..
6	66	$\mu 6_4 2 2$	2	k	show..
7	66	$\mu 6_4 2 2$	5	k	show..

[Click here to see the Series of Maximal Subgroups]

t represents the *translationengleichen* subgroups
k represents the *klassengleichen* subgroups

Figure 1

List of maximal subgroups of the rod group $\mu 6_2 22$ (No. 64) as displayed by the program *MAXSUB*. Subgroups marked as t and k correspond to *translationengleiche* and *klassengleiche* subgroups, respectively. Clicking on ‘show..’ reveals the complete list of subgroups and their distribution in classes of conjugate subgroups (see Fig. 2). The link ‘Click here to see the Series of Maximal Subgroups’ gives direct access to the maximal isotypic subgroups of the rod group $\mu 6_2 22$ (see Fig. 3). Note that the Hermann–Mauguin symbols for rod groups in the BCS do not use the calligraphy font used in *ITE* to depict the Bravais-lattice type.

Maximal k subgroup(s) of type $\mu 6_4 2 2$ (No. 66) of index 2

for rod group $\mu 6_2 22$ (No. 64)

The subgroups of the same type can be divided in conjugacy classes with respect to the subgroup. The transformation matrices of the subgroups in the same conjugacy class are given in the same table.

Click over [ChBasis] to view the general positions of the supergroup in the basis of the subgroup.

Conjugacy class a		
Subgroup(s)	Transformation Matrix	More...
group No 1	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	ChBasis
Conjugacy class b		
Subgroup(s)	Transformation Matrix	More...
group No 2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	ChBasis

Figure 2

Two maximal *klassengleiche* subgroups $\mu 6_1 22$ (No. 63) of index 2 for the rod group $\mu 6_2 22$ (No. 64) obtained by clicking on ‘show..’ in Fig. 1. There are two subgroups for $\mu 6_1 22$ distributed in two conjugacy classes. Note that the Hermann–Mauguin symbols for rod groups in the BCS do not use the calligraphy font used in *ITE* to depict the Bravais-lattice type.

Series of maximal isotypic subgroups of the rod group $p6_2 2 2$ (No. 64)

Series 1
Parametric form of the series 1 of maximal isotypic subgroups of rod group $p6_2 2 2$ (No. 66)

Subgroup	Index	Transformation	Conditions
$p6_2 2 2$ (No. 66)	p	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & p & u \\ 0 & 0 & 0 & 1 \end{bmatrix}$	prime $p > 4$ $p=6n-1$ $0 <= u < p$

Number of conjugate subgroups: p conjugate subgroups

Indices: 5 11 17 23 29 Next

Series 2

Parametric form of the series 2 of maximal isotypic subgroups of rod group $p6_2 2 2$ (No. 64)

Subgroup	Index	Transformation	Conditions
$p6_2 2 2$ (No. 64)	p	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & p & u \\ 0 & 0 & 0 & 1 \end{bmatrix}$	prime $p > 6$ $p=6n+1$ $0 <= u < p$

Number of conjugate subgroups: p conjugate subgroups

Indices: 7 13 19 31 37 Next

Figure 3

Output of the program *MAXSUB* showing the two series of maximal isotypic subgroups for the rod group $p6_2 2 2$ (No. 64). Since the rod group $p6_2 2 2$ belongs to one of the eight pairs of enantiomorphic rod groups, the subgroup of Series 1 corresponds to its enantiomorphic pair $p6_4 2 2$ (No. 66). When the user clicks on the indices below the tables, the program is able to generate the maximal isotypic subgroups for the chosen index (see Fig. 4). Note that the Hermann–Mauguin symbols for rod groups in the BCS do not use the calligraphy font used in *ITE* to depict the Bravais-lattice type.

For certain applications, it is necessary to represent the subgroups \mathcal{H} as subsets of the elements of \mathcal{S} . This is achieved by the option ‘*ChBasis*’ (see Fig. 2), which transforms the general position of \mathcal{H} to the coordinate system of \mathcal{S} .

Maximal subgroups of index higher than 4 have indices p for frieze and rod groups, and p and p^2 for layer groups, where p is a prime. These are isotypic subgroups and are infinite in number. In most of the series, the Hermann–Mauguin symbol for each isotypic subgroup is the same. However, if the subperiodic group belongs to a pair of enantiomorphic groups, the Hermann–Mauguin symbol of the isotypic subgroup is either that of the group or that of its enantiomorphic pair (see Fig. 3). Note that among the subperiodic groups there are only eight pairs of enantiomorphic rod groups: $p4_1$ (No. 24), $p4_3$ (No. 26); $p4_1 2 2$ (No. 31), $p4_3 2 2$ (No. 33); $p3_1$ (No. 43), $p3_2$ (No. 44); $p3_1 1 2$ (No. 47), $p3_2 1 2$ (No. 48); $p6_1$ (No. 54), $p6_5$ (No. 58); $p6_2$ (No. 55), $p6_4$ (No. 57); $p6_1 2 2$ (No. 63), $p6_5 2 2$ (No. 67); and $p6_2 2 2$ (No. 64), $p6_4 2 2$ (No. 66).

There is a link in the program *MAXSUB* (see Fig. 1) that gives direct access to the series of maximal isotypic subgroups of subperiodic groups. Apart from the parametric descriptions of the series, the program provides the individual listing of all maximal isotypic subgroups. The series of maximal isotypic subgroups are shown in blocks grouped by the index and the transformation matrix–column pair (\mathbf{P} , \mathbf{p}) (see Fig. 3). For each series, the Hermann–Mauguin symbol of the subgroup, the restrictions on the parameters describing the series, and the transformation matrix (\mathbf{P} , \mathbf{p}) relating the group \mathcal{S} and the subgroup \mathcal{H} are listed. As an example, Fig. 3 shows the output of maximal isotypic subgroups for the rod-group type $p6_2 2 2$ (No. 64), which is subdivided into two series. There is a special

Maximal isotypic subgroups of type $p6_4 2 2$ (No. 66) of index 5

for the rod group $p6_2 2 2$ (No. 64)

Click over [**ChBasis**] to view the general positions of the subgroup in the basis of the subgroup.

Conjugacy class a		
Subgroup(s)	Transformation Matrix	More...
group No 1	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 5 & 0 \end{pmatrix}$	<input type="button" value="ChBasis"/>
group No 2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 5 & 1 \end{pmatrix}$	<input type="button" value="ChBasis"/>
group No 3	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 5 & 2 \end{pmatrix}$	<input type="button" value="ChBasis"/>
group No 4	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 5 & 3 \end{pmatrix}$	<input type="button" value="ChBasis"/>
group No 5	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 5 & 4 \end{pmatrix}$	<input type="button" value="ChBasis"/>

Figure 4

Complete list of the series of maximal isotypic subgroups $p6_4 2 2$ (No. 66) of index 5 for the rod group $p6_2 2 2$ (No. 64) generated by the auxiliary tool of the program *MAXSUB* (see Fig. 3). Note that the Hermann–Mauguin symbols for rod groups in the BCS do not use the calligraphy font used in *ITE* to depict the Bravais-lattice type.

tool that permits the online generation of maximal isotypic subgroups of any allowed index. Fig. 4 shows the series of maximal isotypic subgroups $p6_4 2 2$ (No. 66) of index 5 for the rod-group type $p6_2 2 2$ (No. 64) generated by this auxiliary tool.

5. Differences between Litvin’s book and the BCS maximal subgroups of subperiodic groups database

Litvin’s book gives the complete listing of the maximal subgroups \mathcal{H} of subperiodic groups \mathcal{S} of indices up to 4. For each maximal subgroup $\mathcal{H} < \mathcal{S}$, the Hermann–Mauguin symbol, the index, the transformation relating the setting of the subperiodic group \mathcal{S} to the setting of the group \mathcal{H} and the coset representatives (in Seitz notation) of the coset decomposition of \mathcal{S} relative to \mathcal{H} are specified. Note that in Litvin’s book the standard International Union of Crystallography Seitz notation is not followed, e.g. a twofold rotation around the c axis is denoted by 2_z instead of 2_{001} [for details cf. Litvin & Kopský (2014)].

The maximal subgroups of subperiodic groups of indices up to 4 of the BCS were compared with a subset of the tables in Litvin’s book. As a result of this comparison, some differences were detected for the maximal subgroups of rod and layer groups; no differences were found for frieze groups. Several errors were identified in Litvin’s book (for more details, see Tables 3 to 6). This list of discrepancies was reviewed with D. Litvin, who has acknowledged them (Litvin, personal communication).

5.1. Transformation matrix (\mathbf{P} , \mathbf{p}) relating the basis of \mathcal{S} and \mathcal{H}

The main difference between Litvin’s book and the BCS is in the transformation matrix–column pair (\mathbf{P} , \mathbf{p}) relating the

Table 3

Typographical errors found in Litvin's book related to the transformation matrix–column pairs (\mathbf{P}, \mathbf{p}) of the maximal subgroups of rod and layer groups.

The subgroups marked with t correspond to *translationengleiche* subgroups.

Group	Subgroup	Index	Type	(\mathbf{P}, \mathbf{p})
$\rho\bar{3}1m$ (No. 51)	$\rho 2/m11$ (No. 6)	3	t	$\mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{b}, \mathbf{c}; 0, 0, 0$
$\rho 6_322$ (No. 65)	$\rho 222_1$ (No. 14)	3	t	$\mathbf{b}, -2\mathbf{a} - \mathbf{b}, \mathbf{b}, \mathbf{c}; 0, 0, 1/4$
$\rho 6_3/mmc$ (No. 75)	$\rho 6_322$ (No. 65)	2	t	$\mathbf{a}, \mathbf{a} + 2\mathbf{b}, \mathbf{a}, \mathbf{c}; 0, 0, 0$
$p\bar{6}2m$ (No. 79)	$cm2m$ (No. 35)	3	t	$\mathbf{a}, \mathbf{a} + 2\mathbf{b}, -\mathbf{a}, \mathbf{c}; 0, 0, 0$

basis of the subperiodic group \mathcal{S} with the subgroup \mathcal{H} . Note that different transformation matrices might specify the *same* (identical) subgroup, if these transformation matrices are related by an element of the affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$ of the subgroup \mathcal{H} . In other words, two subgroups of the same type \mathcal{H}_1 and \mathcal{H}_2 of \mathcal{S} defined by the transformation matrix–column pairs $(\mathbf{P}_1, \mathbf{p}_1)$ and $(\mathbf{P}_2, \mathbf{p}_2)$ are identical if there is an element (\mathbf{N}, \mathbf{n}) of the affine normalizer of the subgroup \mathcal{H} such as

$$(\mathbf{P}_1, \mathbf{p}_1) = (\mathbf{P}_2, \mathbf{p}_2)(\mathbf{N}, \mathbf{n}) \implies (\mathbf{P}_2, \mathbf{p}_2)^{-1}(\mathbf{P}_1, \mathbf{p}_1) = (\mathbf{N}, \mathbf{n}) \in \mathcal{N}_{\mathcal{A}}(\mathcal{H}). \quad (1)$$

The Euclidean and affine normalizers of subperiodic groups are tabulated and available from VanLeeuwen *et al.* (2015).

As an example, let us consider the maximal subgroup $c222$ (No. 22) of index 2 of the layer group $p42_12$ (No. 54). The transformation matrices describing this group–subgroup relation in Litvin's book and the BCS are $(\mathbf{P}, \mathbf{p})_{\text{Litvin}} = \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}; \frac{1}{2}, 0, 0$ and $(\mathbf{P}, \mathbf{p})_{\text{BCS}} = \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}; 0, \frac{1}{2}, 0$, respectively. The affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$ of the layer group $c222$ ($\mathbf{a}, \mathbf{b}, \mathbf{c}$) is the space group $p4/mmm$ with basis vectors $(1/2\mathbf{a}, 1/2\mathbf{b}, \mathbf{c})$. Applying equation (1), the translation $t(0, \frac{1}{2}, 0)$ is obtained. Since $t(0, \frac{1}{2}, 0)$ is an element of the affine normalizer of $c222$, the transformation matrices $(\mathbf{P}, \mathbf{p})_{\text{Litvin}} = \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}; \frac{1}{2}, 0, 0$ and $(\mathbf{P}, \mathbf{p})_{\text{BCS}} = \mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, \mathbf{c}; 0, \frac{1}{2}, 0$ are equivalent and thus describe the *same* identical subgroup.

In general, the differences in (\mathbf{P}, \mathbf{p}) are due to the use of different conventions. For the maximal subgroups of rod groups belonging to trigonal or hexagonal groups with two descriptions in *ITE*, Litvin's book prefers the use of the transformation $2\mathbf{a} + \mathbf{b}, -\mathbf{a} + \mathbf{b}, \mathbf{c}; 0, 0, 0$ (found as the first option in Table 1.2.6.3 of *ITE*), while the BCS prefers the transformation $-\mathbf{a} - 2\mathbf{b}, 2\mathbf{a} + \mathbf{b}, \mathbf{c}; 0, 0, 0$ (second option in Table 1.2.6.3 of *ITE*). In the case of layer groups with two origins, these are described with respect to *origin choice 1* in Litvin's book and *origin choice 2* in the BCS. Therefore, the information on maximal subgroups in these cases differs, since the information provided by these two sources corresponds to different settings.

5.2. List of errors found in Litvin's book

As a result of the comparison of the two sources, a few errors were detected in the description of the maximal subgroups of rod and layer groups in Litvin's book. Three types of errors were identified: (i) typographical errors (see Table 3), (ii) missing subgroups (see Table 4) and (iii) invalid

Table 4

List of the missing maximal subgroups of rod groups $\rho\bar{4}2m$ (No. 37) and $\rho 6_222$ (No. 64) in Litvin's book.

Subgroups marked with t are *translationengleiche* and those marked with k are *klassengleiche*.

Group	Subgroup	Index	Type	(\mathbf{P}, \mathbf{p})
$\rho\bar{4}2m$ (No. 37)	$\rho\bar{4}2m$ (No. 37)	2	k	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 1/2$
$\rho 6_222$ (No. 64)	$\rho 6_422$ (No. 66)	2	k	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 1/2$
$\rho 6_222$ (No. 64)	$\rho 222$ (No. 13)	3	t	$-\mathbf{a} + \mathbf{b}, -\mathbf{a} - \mathbf{b}, \mathbf{c}; 0, 0, 1/3$ $-\mathbf{a} - 2\mathbf{b}, \mathbf{a}, \mathbf{c}; 0, 0, 0$ $2\mathbf{a} + \mathbf{b}, \mathbf{b}, \mathbf{c}; 0, 0, 1/6$

transformation matrix–column pairs (\mathbf{P}, \mathbf{p}) (see Tables 5 and 6).

5.2.1. Typographical errors

Several typographical errors were found in the transformation matrices (\mathbf{P}, \mathbf{p}) relating the subgroup $cm2m$ (No. 35) of the layer group $p\bar{6}2m$ and the subgroups $\rho 2/m11$ (No. 6), $\rho 222_1$ (No. 14) and $\rho 6_322$ (No. 65) of the rod groups $\rho\bar{3}1m$ (No. 51), $\rho 6_322$ and $\rho 6_3/mmc$ (No. 75), respectively. In these cases, four entry transformation matrices are provided (see Table 3) to relate the bases of these groups with their maximal subgroups. These are clear typographical errors in Litvin's book.

Another typographical error can be found in the Hermann–Mauguin symbol of the only maximal subgroup of index 3 of the layer group $pm2_1b$ (No. 28). This subgroup corresponds to an isotypic subgroup of the group $pm2_1b$; therefore, the symbol of the subgroup cannot be $pm2m$ (No. 25) but should be $pm2_1b$.

5.2.2. Missing subgroups

Among the maximal subgroups listed in Litvin's book for the 80 layer, 75 rod and seven frieze groups, only a total of five maximal subgroups are missing for the rod groups $\rho\bar{4}2m$ (No. 37) and $\rho 6_222$ (No. 64) (*cf.* Table 4). There are two maximal subgroups $\rho\bar{4}2m$ of index 2 for the rod group $\rho\bar{4}2m$:

$$[2] \mathbf{c}' = 2\mathbf{c}.$$

$$\rho\bar{4}2m \text{ (No. 37) } \mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 0.$$

$$\rho\bar{4}2m \text{ (No. 37) } \mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 1/2.$$

In Litvin's book, however, only the maximal subgroup with transformation matrix $\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 0$ is listed. For the rod group $\rho 6_222$, there are also two maximal subgroups $p6_422$ (No. 66) of index 2:

$$[2] \mathbf{c}' = 2\mathbf{c}.$$

$$\rho 6_422 \text{ (No. 66) } \mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 0.$$

$$\rho 6_422 \text{ (No. 66) } \mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 1/2.$$

In this case, the subgroup with transformation matrix $\mathbf{a}, \mathbf{b}, 2\mathbf{c}; 0, 0, 1/2$ is not mentioned. The three conjugated subgroups $\rho 222$ (No. 13) of the rod group $\rho 6_222$ of index 3 are also missing from Litvin's book.

5.2.3. Invalid transformation matrix–column pairs (\mathbf{P}, \mathbf{p})

Several cases can be found in Litvin's book in which either the linear part \mathbf{P} or the origin shift \mathbf{p} of the transformation matrix–column pair (\mathbf{P}, \mathbf{p}) relating the basis of the group with

Table 5

Maximal subgroups of rod and layer groups and their corresponding transformation matrices (**P**, **p**) as listed in Litvin's book, whose origin shift **p** is invalid.

The valid origin shift **p_{valid}** is given in the last column of the table. Subgroups marked with *t* are *translationengleiche* and those marked with *k* are *klassengleiche*.

Group	Subgroup	Index	Type	P	p	P_{valid}
μ_6322 (No. 65)	μ_222_1 (No. 14)	3	<i>t</i>	a, a + 2b, c	0, 0, 1/4	0, 0, 0
μ_6c2 (No. 72)	μ_6 (No. 59)	2	<i>t</i>	a, b, c	0, 0, 1/4	0, 0, 0
	μ_312 (No. 46)			a, b, c	0, 0, 0	0, 0, 1/4
μ_6/mcc (No. 74)	μ_6c2 (No. 72)	2	<i>t</i>	a, b, c 2a + b, -a + b, c	0, 0, 1/4 0, 0, 1/4	0, 0, 0 0, 0, 0
μ_63/mmc (No. 75)	μ_6322 (No. 65)	2	<i>t</i>	a, a + 2b, a, c	0, 0, 1/4	0, 0, 0
<i>pb2b</i> (No. 30)	<i>pb2n</i> (No. 34)	2	<i>k</i>	2a, b, c	1, 0, 0	1/2, 0, 0
<i>p4/nbm</i> (No.62)	<i>cmme</i> (No. 48)	2	<i>t</i>	a - b, a + b, c	1/4, 1/4, 0	0, 0, 0

Table 6

List of the maximal subgroups of rod groups and their corresponding transformation matrices (**P**, **p**) as listed in Litvin's book, whose linear part **P** is invalid.

The correct linear part **P_{valid}** is given in the last column of the table. Subgroups marked with *t* are *translationengleiche* and those marked with *k* are *klassengleiche*.

Group	Subgroup	Index	Type	P	p	P_{valid}
μ_4122 (No. 31)	μ_4322 (No. 33)	3	<i>k</i>	a, b, c a, b, c a, b, c	0, 0, 0 0, 0, 1 0, 0, 2	a, b, 3c a, b, 3c a, b, 3c
μ_31c (No. 52)	μ_31c (No. 50, μ_3c1)	2	<i>t</i>	a + b, -a + b, c	0, 0, 0	-a - 2b, 2a + b, c
μ_31c (No. 52)	μ_112/c (No. 7, $\mu_2/c11$)	3	<i>t</i>	a + b, b, c	0, 0, 0	-2a - b, -b, c
μ_6 (No. 53)	μ_112 (No. 8)	3	<i>t</i>	b, c, a	0, 0, 0	a, b, c
μ_63 (No. 56)	μ_112_1 (No. 9)	3	<i>t</i>	b, c, a	0, 0, 0	a, b, c

the subgroup are not valid (see Tables 5 and 6). A non-zero origin shift **p** ≠ (0, 0, 0) is defined in Litvin's book for the transformation matrix relating the maximal subgroup *cmme* (No. 48) of the layer group *p4/nbm* (No. 62) and the maximal subgroups μ_222_1 (No. 14), μ_6 (No. 59), μ_6c2 (No. 72) and μ_6322 (No. 65) of the rod groups μ_6322 (No. 65), μ_6c2 (No. 72), μ_6/mcc (No. 74) and μ_63/mmc (No. 75), respectively. The non-zero origin shifts shown in Table 5 (column six) are not valid, since they do not properly describe their corresponding group–maximal-subgroup relation. In all these cases, it is necessary to have an origin shift **p** = (0, 0, 0). The transformation matrix relating the maximal subgroup μ_312 (No. 46) with the rod group μ_6c2 , defined in Litvin's book with a zero origin shift, is also not valid. The problem is again in the origin shift, which instead of zero is **p** = (0, 0, 1/4). The origin shift of the transformation matrix describing the relation between the maximal subgroup *pb2b* (No. 30) of the layer group *pb2n* (No. 34) is not **p** = (1, 0, 0), but **p** = (1/2, 0, 0).

There are only a few maximal subgroups of rod groups in Litvin's book in which the linear part **P** of the transformation matrix is not correctly defined (see Table 6). The transformation matrix (**P**, **p**)_{Litvin} = (**b, c, a**; 0, 0, 0), provided by Litvin's book, describes the relationship between the maximal subgroups μ_112 (No. 8) and μ_112_1 (No. 9) of index 3 of the rod groups μ_6 (No. 53) and μ_63 (No. 56), respectively. This transformation matrix results in different maximal subgroups: μ_211 for μ_6 , and μ_2111 for μ_63 (No. 53). The valid transformation matrix for these cases requires a linear part **P** equal to the identity matrix, i.e. **P** = **a, b, c**. The linear part **P** of the transformation matrix–column pairs of the three conjugated

maximal subgroups μ_4322 (No. 33) of index 3 for rod group μ_4122 (No. 31), defined in Litvin's book as **a, b, c**, is also not valid. In this particular case, the correct **P** is **a, b, 3c**. Similar problems (see Table 6) can also be found for the maximal subgroups μ_3c1 (No. 50) and $\mu_2/c11$ (No. 7) of index 3 and 2 of the rod group μ_31c (No. 52).

6. Conclusions

The Bilbao Crystallographic Server offers the only complete and freely accessible database of maximal subgroups of subperiodic groups through the program *MAXSUB*. This program provides detailed information on both maximal non-isotypic and isotypic subgroups with indices up to 9, along with series of maximal isotypic subgroups.

A thorough comparison with the existing reference by Litvin (2013) has been conducted, revealing several discrepancies (which are analysed). These findings underscore the completeness of the BCS data, reinforcing their value as the most comprehensive resource for crystallographic research and subgroup analysis.

APPENDIX A

Types of subgroups of subperiodic groups

On the basis of Hermann's theorem (Hermann, 1929) for space groups, the following types of subgroups of subperiodic groups can be distinguished:

(i) A subgroup \mathcal{H} of a subperiodic group \mathcal{S} is called a *translationengleiche* subgroup or a *t* subgroup of \mathcal{S} if the set

\mathcal{T}_S of translations is retained, i.e. $\mathcal{T}_\mathcal{H} = \mathcal{T}_S$, but the order of the point group \mathcal{P}_S is reduced.

(ii) A subgroup $\mathcal{H} < \mathcal{S}$ of a subperiodic group \mathcal{S} is called a *klassengleiche* subgroup or a *k* subgroup if the set \mathcal{T}_S of all translations of \mathcal{S} is reduced to $\mathcal{T}_\mathcal{H} < \mathcal{T}_S$ but the point group $\mathcal{P}_\mathcal{H}$ is the same as that of \mathcal{P}_S .

(iii) A *klassengleiche* or *k* subgroup $\mathcal{H} < \mathcal{S}$ is called an isotypic subgroup if it belongs to the same affine subperiodic group as \mathcal{S} .

(iv) A subgroup of a subperiodic group $\mathcal{H} < \mathcal{S}$ is called *general* or a *general subgroup* if it is neither a *translationengleiche* nor a *klassengleiche* subgroup, i.e. $\mathcal{T}_\mathcal{H} < \mathcal{T}_S$ and $\mathcal{P}_\mathcal{H} < \mathcal{P}_S$.

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