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Nomenclature of Polytype Structures

Report of the International Union of Crystallography *Ad-Hoc* Committee on the Nomenclature of Disordered, Modulated and Polytype Structures*

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Abstract

An earlier report [*Acta Cryst.* (1977), A**33**, 681–684] by a joint IUCr–IMA committee on the nomenclature of polytypism has been revised and extended. Two kinds of symbolism are recommended for use with either simple or complicated polytypic structures. The first consists of 'indicative symbols' in a modified Gard notation, the second of 'descriptive symbols' based on earlier proposals by Dornberger-Schiff, Ďurovič and Zvyagin. The polytypism of ZnS and $SrGeO_3$ provides examples for the use of descriptive symbolism.

Introduction

This report is concerned exclusively with the nomenclature of polytype structures. An earlier recommendation on polytype nomenclature was published in *Acta Cryst.* (1977), A**33**, 681–684 by a joint IUCr–IMA committee. In part III of that recommendation, a new symbolism that was based on the work of Dornberger-Schiff & Ďurovič (1974) and Zvyagin (1967, 1974) was proposed but not given in detail. The present report gives a full description of these symbols in § II.2 as approved by the *Ad-Hoc* Committee. For completeness, the basic 1977 recommendations are included in §§ I and II.1 in modified form.

I. Definition

An element or compound is *polytypic* if it occurs in several different structural modifications, each of which may be regarded as built up by stacking layers of (nearly) identical structure and composition, and if the modifications differ only in their stacking sequence. Polytypism is a special case of polymorphism: the two-dimensional translations within the layers are (essentially) preserved whereas the lattice spacings normal to the layers vary between polytypes and are indicative of the stacking period. No such restrictions apply to polymorphism.

Comment: The above definition is designed to be sufficiently general to make polytypism a useful concept. There is increasing evidence that some polytypic structures are characterized either by small deviations from stoichiometry or by small amounts of impurities. (In the case of certain minerals like clays, micas and ferrites, deviations in composition up to 0·25 atoms per formula unit are permitted within the same polytypic series: two layer structures that differ by more

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* Appointed in 1979 by the IUCr Executive Committee under ground rules outlined in *Acta Cryst.* (1979). A35, 1072. Final Report accepted in 1983 by the IUCr Commission on Crystallographic Nomenclature and the Executive Committee.

† The major contributions made by K. Boll-Dornberger to this Report until her death in July 1981 are deeply appreciated.

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than this amount should not be called polytypic.) Likewise, layers in different polytypic structures may exhibit slight structural differences and may not be isomorphic in the strict crystallographic sense.

The *Ad-Hoc* Committee is aware that the definition of polytypism above is probably too wide since it includes, for example, the turbostratic form of graphite as well as mixed-layer phyllosilicates. However, the sequence and stacking of layers in a polytype are always subject to well-defined limitations. On the other hand, a more general definition of polytypism that includes 'rod' and 'block' polytypes may become necessary in the future.

General recommendations concerning names commonly used in the studies of polytypic materials are given in the 1977 report.

II. Polytype symbolism

The *Ad-Hoc* Committee has examined the systems of structural symbols for polytypic structures already in the literature, which may be divided into two categories:

the first, of *indicative symbols*, includes systems that can be used without knowledge of the crystal structure; these necessarily make use of observable characteristics such as symmetry, periodicity of layers, interchange of axes, *etc.*;

the second, of *descriptive symbols*, includes systems that specify the exact stacking sequence of layers. Such systems allow the reader to deduce the unit cell and space group, and to recognize identical structures described by different axes or unit cells (settings); they facilitate comparison of structural data referring to different polytypes and allow identification by means of calculated intensities.

Most notational systems in the literature have been designed specifically for certain types of structure and, in the opinion of the *Ad-Hoc* Committee, cannot be applied universally. Several systems that showed promise were examined in more detail and have been further modified.

The *Ad-Hoc* Committee approves the system recommended in 1977 for the first category, see § II.1, and recommends the system described in § II.2 for the second category.

II.1. *Indicative symbols*: *modified Gard notation*

Gard (1966) has described a nomenclature for fibrous calcium silicates that was modified by A. Kato and H. Schulz in the 1977 report. The modified Gard notation is recommended here because it takes into account multiple translation periods along all three axes as well as the interchange of axes relative to a standard subcell. For polytypes without interchange of axes and with multiple periodicity normal only to the layers, a simplified version of the notation may be used which is similar to that introduced by Ramsdell (1947) for SiC and is in common use for phyllosilicates. Although the modified Gard notation has been adapted here to describe polytype structures, it is evident from the examples considered below that it can also be useful in nonpolytypic cases involving permutations of axes or superstructures in one or more directions.

In this system the symbol to describe a polytypic phase consists of a mineral name and an italicized supplement, combined by a hyphen. The supplement contains four positions, with additional marks when necessary. The first position in the symbol is filled by one of the following capital letters to indicate the crystal system of the compound:*

cubic = *C*
hexagonal = *H*
trigonal (with hexagonal Bravais lattice) = *T*
trigonal (with rhombohedral Bravais lattice) = *R*
tetragonal (quadratic) = *Q*
orthorhombic = *O*
monoclinic = *M*
triclinic (anorthic) = *A*.

Three lower-case letters, accompanied by numbers when necessary, follow the symmetry symbol to indicate the periodicities along the three axes (in the order *a*, *b*, *c*) of the compound relative to those of the smallest subcell of the polytypic system. Thus, molybdenite-2*H* is written as molybdenite-*Haa*2*c* and molybdenite-3*R* as molybdenite-*Raa*3*c*. In cases where the pseudosymmetry is of special interest, the letter ψ (abbreviation of *pseudo-*) is added before the symmetry symbol. For example, ψH means pseudo-hexagonal. Thus, pearceite is written as pearceite-$\psi Habc$ and arseno-polybasite as pearceite-$\psi H2a2b2c$. The permutation of axes relative to that of the parent-structure subcell is easily indicated by permuting the appropriate symbols, for example (see Appendix 1), gibbsite-$\psi Oabc$ and gibbsite-$\psi M2b2ac$. A definition of these species has been given by Strunz (1966).

In order to distinguish the ordered and disordered polytypes of xonotlite, described by Gard (1966) as $P121$ and $P\infty21$, both of which are $Ma2bc$ or $\psi Oa2bc$ in the proposed system, an additional symbol *d* (abbreviation for disordered) is added as a subscript to the letter involved. That is, $P\infty21$ is written as Ma_d2bc or ψOa_d2bc.

In order to reconcile the present notation with that of Ramsdell, the following simplification may be made. If the four-position symbol describes a tetragonal or hexagonal compound, then the first two

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* The *Ad-Hoc* Committee is aware that this notation does not conform with that of *International Tables for Crystallography* (1983) or *Structure Reports* but recommends its retention since it is embedded in the literature. It is, however, recommended that use of these symbols be confined exclusively to polytype description terminology.

axes have the same length, as in graphite-*Haa*2*c*. In this case, it is permissible to delete the first two axes and place the periodicity of the third axis in front of the capital letter symbolizing the crystal system. Thus graphite-*Haa*2*c* becomes graphite-2*H*. This rule is also applicable to polytypes with pseudo-hexagonal symmetry. In this case, the deleted letters are not always *aa* but may be *bc*, *ab*, *ba*, *etc.*, where $b = a\surd 3$. Thus, indialite may be given as cordierite-1*H* and cordierite (*sensu stricto*) as cordierite-1*O* or cordierite-1ψ*H*.

In the case of the polytypic micas, $2M_1$ and $2M_2$ require different treatment. Thus, muscovite-$2M_1$ = muscovite-*Mab*2*c* or -ψ*Hab*2*c* can be shortened to muscovite-2*M* or -2ψ*H*. But for muscovite-$2M_2$ = muscovite-*Mba*2*c* or -ψ*Hba*2*c*, the long symbol should be retained if the reversal of two axes is to be described. This system, however, is not intended to replace symbols such as $2M_1$ and $2M_2$ that are useful and internationally accepted.

Examples of the recommended nomenclature are given in Appendix 1 for a representative number of mineral groups. The mineral names tabulated are chosen for familiarity and are intended to be illustrative, rather than exhaustive, and cover related phases by the least number of names. The *Ad-Hoc* Committee does not necessarily recommend that all traditional names be dropped. Polytypic non-minerals are to be referred to by their chemical formula and appropriate supplement.

II.2. *Descriptive symbols*: *notation*

In certain polytypic compounds a number of different polytypic structures may have an identical modified Gard symbol. A more detailed symbolism is hence desirable to allow specification of the exact stacking sequence of layers, if known. Such detailed symbols are necessarily complex, and the ideal goal is a symbol that gives the necessary information in a readily understandable format. Too complex a symbol will probably be used only by a few experts in the field.

In the present recommendation, the stacking sequence of two-dimensionally periodic *building layers* (BLs) in any polytype is described by a sequence of conventionally chosen characters (numbers, letters, signs, *etc.*) which indicate the *absolute orientation* of each BL and the *relative displacements* of their origins. Before presenting the symbols for a given polytypic family, the choice of BLs, their origins, possible orientations and stacking possibilities are to be specified – *e.g.* by indicating the *orientational and displacement vectors* in diagrams of the normal projection of the structure onto the plane parallel to the BLs relative to a fixed coordinate system. The choice of orientational and displacement characters and other relevant items should also be given in this *explanatory introduction.*

The orientational characters should be in upper-case and the displacement characters in lower-case letters (denoting different kinds of BLs and structural displacements, respectively): both may have subscripts [integer numbers, sign (+, −), *etc.*], chosen by convention, to indicate respective orientation and displacement. The sequence of BLs is hence given by a corresponding sequence of *orientational* and *displacement characters*, as in (1).

$$\ldots P_i s_j Q_k t_l R_m u_n \ldots . \qquad (1)$$

If the BLs are all equivalent, *or* if their nature, orientation (and/or displacement) is fixed or otherwise obvious, the letters ... *P*, *Q*, *R*, ... (... *s*, *t*, *u*, ...) may be omitted and only their subscripts used as orientational and displacement characters. These are generally written in a two-line form with orientation characters in the upper and displacement characters in the lower line. In this case, symbol (1) becomes

$$\ldots {}^{i}{}_{j}{}^{k}{}_{l}{}^{m}{}_{n} \ldots . \qquad (2)$$

If the orientations (displacements) are all alike, or if they follow unambiguously from displacements (orientations), the corresponding characters may be omitted. In such a case, sequence (1) may be reduced to

$$\ldots s_j t_l u_n \ldots (\ldots P_i Q_k R_m \ldots). \qquad (3)$$

An analogous reduction is also possible for sequence (2):

$$\ldots jln \ldots (\ldots ikm \ldots). \qquad (4)$$

Characters which are redundant may or may not be omitted, and accordingly we speak of *non-redundant* and *redundant symbols*, respectively. A symbol may also contain additional marks (dots, primes, *etc.*) for facilitating the recognition of relevant crystal-chemical features. The smallest repeating part of the periodic sequence of characters, placed between vertical bars (|...|) indicates periodic polytypes. The number of BL-repeating units per symbol-repeating unit is represented by the corresponding subscript number.

When a polytypic structure consists of equivalent BLs and any BL may occupy only one of two alternative positions relative to the preceding BL, the polytypic symbol is reduced to the simplest form, *i.e.* a sequence of characters of two kinds, *e.g.* + and − in Hägg's (1943) symbolism, which in turn is simplified to the short-hand form of Zhdanov's (1945) symbolism, indicating the numbers *m* and *n* of the consecutive characters + and −, respectively.

Examples of recommended descriptive symbols are given in Appendix 2. Additional details may be found in Dornberger-Schiff, Ďurovič & Zvyagin (1982).

It is a pleasure to thank A. J. C. Wilson for improving this report by his critical comments.

APPENDIX 1

Examples of the application of the modified Gard nomenclature to some representative mineral groups, followed by traditional names in parentheses (not all examples are strict polytypes); further examples are given in the 1977 report

Elements
graphite-2*H* (graphite-2*H*)
graphite-3*R* (graphite-3*R*)
Sulphides
sternbergite-*Oab*2*c* (sternbergite)
sternbergite-*Oabc* (argentopyrite)
pyrrhotite-*Hbbc* (troilite)
pyrrhotite-*H*2*a*2*a*6*c* (6*C*-type pyrrhotite)
pyrrhotite-*O*2*a*2*b*11*c* (11*C*-type pyrrhotite)
pearceite-*ψHaac* (pearceite)
pearceite-*ψH*2*a*2*a*2*c* (arsenopolybasite)
andorite-*Oab*12*c* (andorite)
andorite-*ψOab*24*c* (nakaseite)
Halogenides
atacamite-*R*2*a*2*a*3*c* (paratacamite)
Oxides
taaffeite-4*H* (taaffeite)
taaffeite-9*R*
gibbsite-*ψOabc* (bayerite)
gibbsite-*Mba*2*c* (hydrargillite)
Carbonates
hydrotalcite-2*H* (manasseite)
pyroaurite-3*R* (pyroaurite)
Borates
veatchite-*Ma*2*bc* (veatchite)
Sulphates
coquimbite-3*R* (paracoquimbite)
Phosphates, arsenates, and vanadates
variscite-*ψOabc* (metavariscite)
strengite-*ψOabc* (metastrengite)
Silicates
chloritoid-*Aabc* (chloritoid-1*A*)
zoisite-*Mabc* (clinozoisite)
cordierite-1*H* (indialite)
anthophyllite-*O*2*abc* (anthophyllite)
wollastonite-*Aabc* (wollastonite)
wollastonite-*M*2*abc* (parawollastonite)

APPENDIX 2

Examples of descriptive symbols for some polytypic structures, with dependence on choice of BLs, origins and stacking direction

A. Explanatory introduction and explicit table of symbols for two cases

(1) ZnS *Family*. The structures (see Fig. 1) may be considered to consist of BLs chosen as follows (Verma & Krishna, 1966).

(*a*) Sheets of Zn–S dumb-bells projecting in close-packing positions denoted by *A*, *B*, *C*, with any two successive positions corresponding to different letters. Sequences *AB*, *BC*, *CA* are equivalent and may be considered as displacements q_+; the reverse sequences *AC*, *CB*, *BA* give displacements of opposite sense q_-.

(*b*) Sheets of ZnS_4 tetrahedra sharing common corners. The displacements of these BLs are characterized by the same sequences as above and also serve as orientational vectors Q_+ and Q_-. Since the displacement and orientation senses coincide, one kind of character is sufficient for the description.

An example is given in Table 1.

(2) *Strontium germanate*: $SrGeO_3$. Sheets of SrO_6 octahedra (sharing edges, see Fig. 2) are linked by sheets of isolated three-membered rings of GeO_4 tetrahedra: all rings share their non-bridging O atoms with octahedra and project onto every third triangle between the bases of adjacent SrO_6 octahedra (Dornberger-Schiff, 1961). There are three choices of BLs.

(*a*) Two kinds of BLs, with BL(1) an octahedral sheet and BL(2) a sheet of isolated tetrahedral rings. Non-bridging oxygen ring atoms belong half to one, half to the adjacent BL. Since successive BLs of one kind regularly alternate with respect to their orientations, displacements (between ring centers) only are sufficient to describe the polytypes.

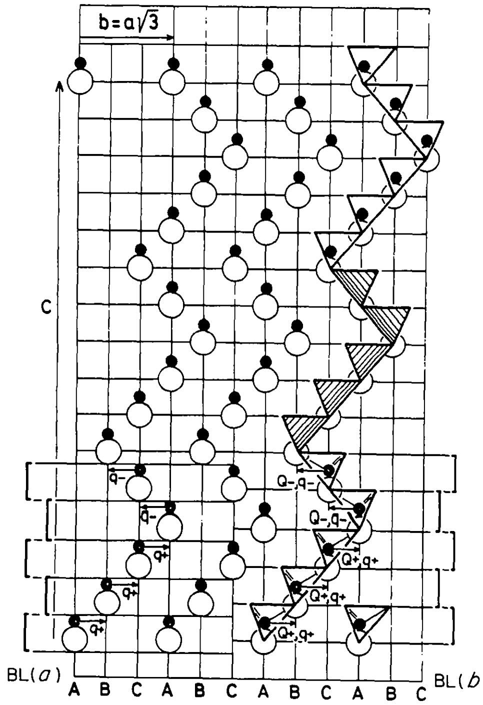


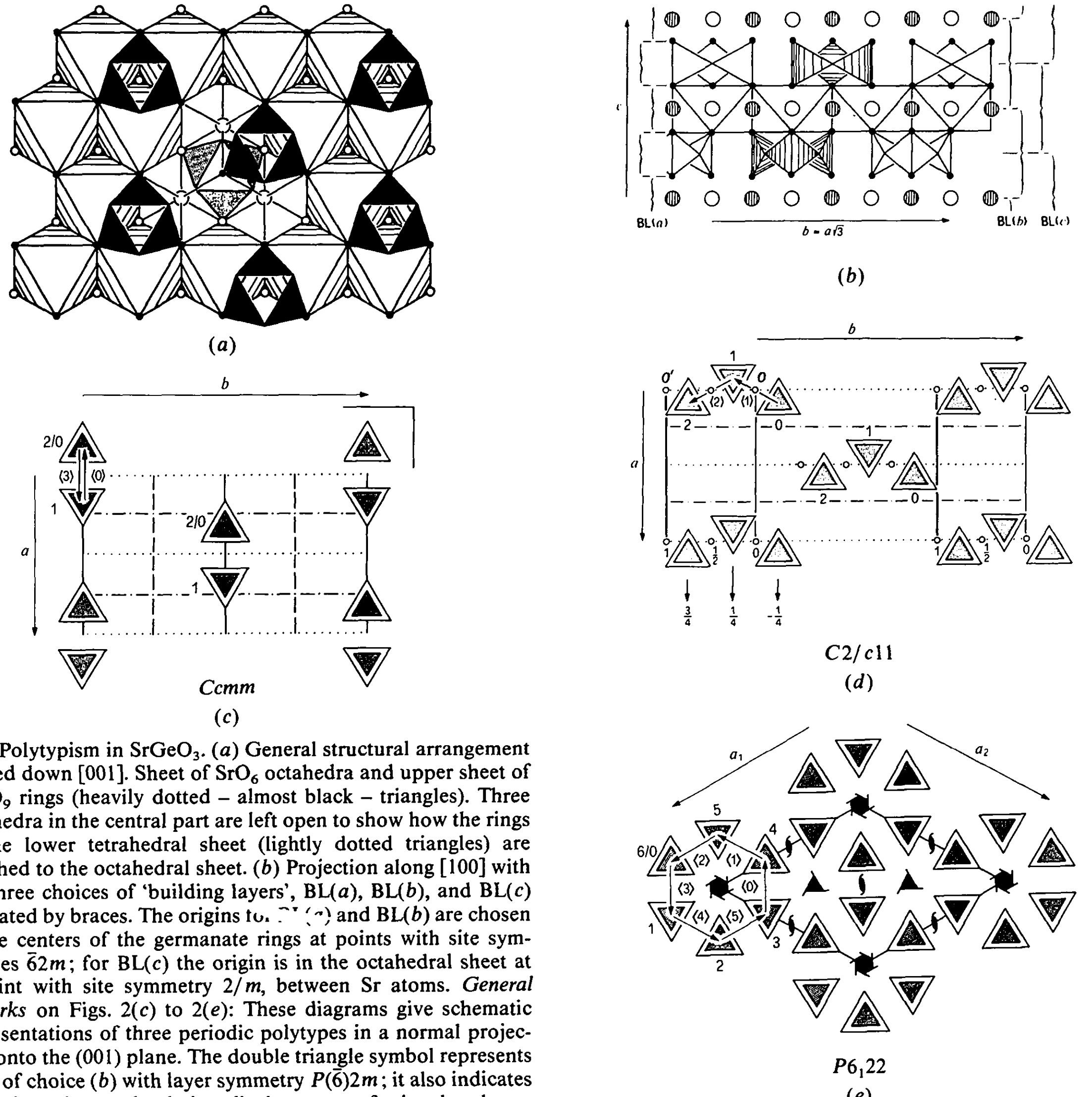
Fig. 1. Polytype 15*R* of ZnS. Structural arrangement in the $(11\bar{2}0)$ section illustrating the orientational and displacement characters for the two choices of BLs. The S atoms of the adjacent sections which belong to the indicated tetrahedra for BL choice (*b*) are not drawn (see Appendix 2). Origins of BLs are chosen at the starting points of arrows indicating their displacements.

Table 1. *Descriptive symbols for* ZnS

Substance	BLs chosen	Full symbol (redundant)	Simplified symbol (nonredundant)	Number of BLs per repeat	Space group
ZnS (15*R*)	(*a*)	$\vert q_+q_+q_+q_-q_-\vert_3$	$\vert +++--\vert_3$	15	*R*3*m*
	(*b*)	$\vert Q_+q_+Q_+q_+Q_+q_+Q_-q_-Q_-q_-\vert_3$			

(*b*) One kind of equivalent BL: germanate sheets with planes of Sr half-atoms attached on either side. Displacements as in (*a*) are used.

(*c*) One kind of equivalent BL: octahedral sheets with planes of Ge and bridging O half-atoms attached to them on either side. Displacement vectors as in (*a*) and (*b*) are to be considered orientational vectors. These vectors have length $a/3$ in the normal projection on the orthohexagonal basis plane *ab* and are related by counterclockwise rotations of $2\pi n/6$ about



(*a*)

(*b*)

Ccmm

(*c*)

*C*2/*c*11

(*d*)

*P*6₁22

(*e*)

Fig. 2. Polytypism in SrGeO$_3$. (*a*) General structural arrangement viewed down [001]. Sheet of SrO$_6$ octahedra and upper sheet of Ge$_3$O$_9$ rings (heavily dotted – almost black – triangles). Three octahedra in the central part are left open to show how the rings of the lower tetrahedral sheet (lightly dotted triangles) are attached to the octahedral sheet. (*b*) Projection along [100] with the three choices of 'building layers', BL(*a*), BL(*b*), and BL(*c*) indicated by braces. The origins for BL(*a*) and BL(*b*) are chosen in the centers of the germanate rings at points with site symmetries $\bar{6}2m$; for BL(*c*) the origin is in the octahedral sheet at a point with site symmetry $2/m$, between Sr atoms. *General remarks* on Figs. 2(*c*) to 2(*e*): These diagrams give schematic representations of three periodic polytypes in a normal projection onto the (001) plane. The double triangle symbol represents a BL of choice (*b*) with layer symmetry $P(\bar{6})2m$; it also indicates the orientation and relative displacement of triangles drawn through the bridging oxygen atoms of the germanate rings. BLs are numbered according to sequence, 2/0 (6/0) means a coincidence of the second (sixth) and zeroth BL in projection. Displacement vectors $\langle j\rangle$ (*j*-displacement character) and some relevant symmetry elements of the respective space groups are also given. (*c*) Orthorhombic polytype |30| projected along [001]; space group *Ccmm*. (*d*) Monoclinic polytype |12|, projected along **c***, which in this case is parallel to [013]; space group *C*2/*c*11 (*a*-axis setting). The *c* axis slopes upwards to the left from the cell origin *0* in the bottom (001) face of the cell to the origin *0'* in the top (001) face, *i.e.* $\mathbf{c}=\mathbf{d}_{001}-\frac{1}{3}\mathbf{b}$. Hence, the *c* components of the glide vectors of the *c* and *n* glides are inclined to the plane of the figure. The triangles 0, 1, 2, ... are related by the successive operations of the *c* glide planes; triangle 6 would project onto triangle 0. (*e*) Hexagonal polytype |345012|, projected along [001]; space group $P6_122$.

Table 2. *Descriptive symbols for* $SrGeO_3$

Substance $SrGeO_3$	BLs chosen	Full symbol (redundant)	Simplified symbol (nonredundant)	Number of equivalent BLs per repeat	Space group
(2*O*)	(*a*)(*b*)	$\lvert p_3p_0\rvert$	|30|	2	*Ccmm*
	(*c*)	$\lvert P_3P_0\rvert$			
(2*M*)	(*a*)(*b*)	$\lvert p_1p_2\rvert$	|12|	2	*C*2/*c*11
	(*c*)	$\lvert P_1P_2\rvert$			
(6*H*)	(*a*)(*b*)	$\lvert p_3p_4p_5p_0p_1p_2\rvert$	|3 4 5 0 1 2|	6	$P6_122$
	(*c*)	$\lvert P_3P_4P_5P_0P_1P_2\rvert$			

the *c* axis. They are accordingly assigned the characters $n=0, 1, \ldots, 5$. The character 0 (or 6) denotes the vector parallel to $-\mathbf{a}$ of the orthogonal *C*-centered base a, $b=a\sqrt{3}$.

An example is given in Table 2.

B. Illustrative papers on polytypic substances with description of symbolism used

Astrophyllite

Zvyagin & Vrublevskaya (1976).

Kaolinite-type structures

Zvyagin (1964, 1967) (tri- and di-octahedral polytypes).

Dornberger-Schiff & Ďurovič (1975) (tri-, di- and mono-octahedral polytypes).

Mica

Zvyagin (1964, 1967) (tri-octahedral polytypes).

Takeda (1967) (tri-octahedral polytypes).

Dornberger-Schiff, Backhaus & Ďurovič (1982) (tri-, di- and mono-octahedral polytypes).

Vermiculites

Weiss & Ďurovič (1980).

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Graphic Representation and Nomenclature of the Four-Dimensional Crystal Classes. III. A Notation for the Crystal Classes

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Abstract

A Hermann–Mauguin type notation is devised for the 227 four-dimensional (geometric) crystal classes, and appropriate conventions are proposed for each of the 23 crystal families.

Introduction

In paper I of the series (Whittaker, 1983) the principle was demonstrated of representing graphically the symmetry of the four-dimensional crystal classes by means of the hyperstereogram. Such representations

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