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3.3. Space-group symbols and their use

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3.3.1. Point-group symbols

3.3.1.1. Introduction

For symbolizing space groups, or more correctly types of space groups, different notations have been proposed. The following three are the main ones in use today:

(i) the notation of Schoenflies (1891, 1923);

(ii) the notation of Shubnikov (Shubnikov & Koptsik, 1972), which is frequently used in the Russian literature;

(iii) the international notation of Hermann (1928*a*) and Mauguin (1931). This was used in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (*IT* 1935) and was somewhat modified in *International Tables for X-ray Crystallography* (*IT* 1952).

In all three notations, the space-group symbol is a modification of a point-group symbol.

Symmetry elements occur in lattices, and thus in crystals, only in distinct directions. Point-group symbols make use of these discrete directions and their mutual relations.

3.3.1.2. Schoenflies symbols

Most Schoenflies symbols (Table 3.3.1.3, column 1) consist of the basic parts C_n, D_n,[1] T or O, designating cyclic, dihedral, tetrahedral and octahedral rotation groups, respectively, with $n = 1, 2, 3, 4, 6$. The remaining point groups are described by additional symbols for mirror planes, if present. The subscripts h and v indicate mirror planes perpendicular and parallel to a main axis taken as vertical. For T, the three mutually perpendicular twofold axes and, for O, the three fourfold axes are considered to be the main axes. The index d is used for mirror planes that bisect the angle between two consecutive equivalent rotation axes, *i.e.* which are diagonal with respect to these axes. For the rotoinversion axes $\bar{1}$, $\bar{2} \equiv m$, $\bar{3}$ and $\bar{4}$, which do not fit into the general Schoenflies concept of symbols, other symbols C_i, C_s, C_{3i} and S_4 are in use. The rotoinversion axis $\bar{6}$ is equivalent to $3/m$ and thus designated as C_{3h}.

A detailed introduction to Schoenflies symbols of crystallographic point groups is given in Section 1.4.1.3.

3.3.1.3. Shubnikov symbols

The Shubnikov symbol is constructed from a minimal set of generators of a point group (for exceptions, see below). Thus, strictly speaking, the symbols represent types of symmetry operations. Since each symmetry operation is related to a symmetry element, the symbols also have a geometrical meaning. The Shubnikov symbols for symmetry operations differ slightly from the international symbols (Table 3.3.1.1). Note that Shubnikov, like Schoenflies, regards symmetry operations of the second kind as rotoreflections rather than as rotoinversions.

If more than one generator is required, it is not sufficient to give only the types of the symmetry elements; their mutual orientations must be symbolized too. In the Shubnikov symbol, a dot (·), a colon (:) or a slash (/) is used to designate parallel, perpendicular or oblique arrangement of the symmetry elements. For a reflection, the orientation of the actual mirror plane is considered, not that of its normal. The exception mentioned above is the use of $3 : m$ instead of $\tilde{3}$ in the description of point groups.

[1] Instead of D_2, in older papers V (from *Vierergruppe*) is used.

3.3.1.4. Hermann–Mauguin symbols

3.3.1.4.1. Symmetry directions

The Hermann–Mauguin symbols for finite point groups make use of the fact that the symmetry elements, *i.e.* proper and improper rotation axes, have definite mutual orientations. If for each point group the symmetry directions are grouped into classes of symmetry equivalence, at most three classes are obtained. These classes were called *Blickrichtungssysteme* (Heesch, 1929). If a class contains more than one direction, one of them is chosen as representative.

The Hermann–Mauguin symbols for the crystallographic point groups refer to the symmetry directions of the lattice point groups (holohedries, *cf.* Sections 1.3.4.3 and 3.1.1.4) and use other representatives than chosen by Heesch [*IT* (1935), p. 13]. For instance, in the hexagonal case, the primary set of lattice symmetry directions consists of {[001], [00$\bar{1}$]}, representative is [001]; the secondary set of lattice symmetry directions consists of [100], [010], [$\bar{1}\bar{1}$0] and their counter-directions, representative is [100]; the tertiary set of lattice symmetry directions consists of [1$\bar{1}$0], [120], [$\bar{2}\bar{1}$0] and their counter-directions, representative is [1$\bar{1}$0]. The representatives for the sets of lattice symmetry directions for all lattice point groups are listed in Table 3.3.1.2. The directions are related to the conventional crystallographic basis of each lattice point group (*cf.* Section 3.1.1.4).

The relation between the concept of lattice symmetry directions and group theory is evident. The maximal cyclic subgroups of the maximal rotation group contained in a lattice point group can be divided into, at most, three sets of conjugate subgroups. Each of these sets corresponds to one set of lattice symmetry directions.

Table 3.3.1.1
International (Hermann–Mauguin) and Shubnikov symbols for symmetry elements

The first power of a symmetry operation is often designated by the symmetry-element symbol without exponent 1, the other powers of the operation carry the appropriate exponent.

	Symmetry elements	
	of the first kind	of the second kind
Hermann–Mauguin	1 2 3 4 6	$\bar{1}$ m $\bar{3}$ $\bar{4}$ $\bar{6}$
Shubnikov†	1 2 3 4 6	$\tilde{2}$ m $\tilde{6}$ $\tilde{4}$ $\tilde{3}$

† According to a private communication from J. D. H. Donnay, the symbols for elements of the second kind were proposed by M. J. Buerger. Koptsik (1966) used them for the Shubnikov method.

Table 3.3.1.2
Representatives for the sets of lattice symmetry directions in the various crystal families

	Crystal family	Anorthic (triclinic)	Monoclinic	Orthorhombic	Tetragonal	Hexagonal		Cubic
Lattice point group	Schoenflies	C_i	C_{2h}	D_{2h}	D_{4h}	D_{6h}	D_{3d}	O_h
	Hermann–Mauguin	$\bar{1}$	$\frac{2}{m}$	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	$\bar{3}\frac{2}{m}$†	$\frac{4}{m}\bar{3}\frac{2}{m}$
Set of lattice symmetry directions	Primary	–	[010] *b* unique [001] *c* unique	[100]	[001]	[001]	[001]	[001]
	Secondary	–	–	[010]	[100]	[100]	[100]	[111]
	Tertiary	–	–	[001]	[1$\bar{1}$0]	[1$\bar{1}$0]	–	[1$\bar{1}$0] [110]‡

† In this table, the directions refer to the hexagonal description. The use of the primitive rhombohedral cell brings out the relations between cubic and rhombohedral groups: the primary set is represented by [111] and the secondary by [1$\bar{1}$0]. ‡ Only for $\bar{4}3m$ and 432 [for reasons see text].

3.3.1.4.2. Full Hermann–Mauguin symbols

After the classification of the directions of rotation axes, the description of the seven maximal rotation subgroups of the lattice point groups is rather simple. For each representative direction, the rotational symmetry element is symbolized by an integer *n* for an *n*-fold axis, resulting in the symbols of the maximal rotation subgroups 1, 2, 222, 32, 422, 622, 432. The symbol 1 is used for the triclinic case. The complete lattice point group is constructed by multiplying the rotation group by the inversion $\bar{1}$. For the even-fold axes, 2, 4 and 6, this multiplication results in a mirror plane perpendicular to the rotation axis yielding the symbols $(2n)/m$ (n = 1, 2, 3). For the odd-fold axes 1 and 3, this product leads to the rotoinversion axes $\bar{1}$ and $\bar{3}$. Thus, for each representative of a set of lattice symmetry directions, the symmetry forms a point group that can be generated by one, or at most two, symmetry operations. The resulting symbols are called *full Hermann–Mauguin (or international) symbols*. For the lattice point groups they are shown in Table 3.3.1.2.

For the description of a point group of a crystal, we use its lattice symmetry directions. For the representative of each set of lattice symmetry directions, the remaining subgroup is symbolized; if only the primary symmetry direction contains symmetry higher than 1, the symbols '1' for the secondary and tertiary set (if present) can be omitted. For the cubic point groups T and T_h, the representative of the tertiary set would be '1', which is omitted. For the rotoinversion groups $\bar{1}$ and $\bar{3}$, the remaining subgroups can only be 1 and 3. If the supergroup is $(2n)/m$, five different types of subgroups can be derived: n/m, $2n$, $\overline{2n}$, n and m. In the cubic system, for instance, $4/m$, $2/m$, $\bar{4}$, 4 or 2 may occur in the primary set. In this case, the symbol m can only occur in the combinations $2/m$ or $4/m$ as can be seen from Table 3.3.1.3.

3.3.1.4.3. Short symbols and generators

If the symbols are not only used for the identification of a group but also for its construction, the symbol must contain a list of generating operations and additional relations, if necessary. Following this aspect, the Hermann–Mauguin symbols can be shortened. The choice of generators is not unique; two proposals were presented by Mauguin (1931). In the first proposal, in almost all cases the generators are the same as those of the Shubnikov symbols. In the second proposal, which, apart from some exceptions (see Section 3.3.4), is used for the international symbols, Mauguin selected a set of generators and thus a list of short symbols in which reflections have priority (Table 3.3.1.3, column 3). This selection makes the transition from the short point-group symbols to the space-group symbols fairly simple. These short symbols contain two kinds of notation components:

Table 3.3.1.3
Point-group symbols

Schoenflies	Shubnikov	*International Tables*, short symbol	*International Tables*, full symbol
C_1	1	1	1
C_i	$\tilde{2}$	$\bar{1}$	$\bar{1}$
C_2	2	2	2
C_s	m	m	m
C_{2h}	$2 : m$	$2/m$	$2/m$
D_2	$2 : 2$	222	222
C_{2v}	$2 \cdot m$	$mm2$	$mm2$
D_{2h}	$m \cdot 2 : m$	mmm	$2/m\ 2/m\ 2/m$
C_4	4	4	4
S_4	$\tilde{4}$	$\bar{4}$	$\bar{4}$
C_{4h}	$4 : m$	$4/m$	$4/m$
D_4	$4 : 2$	422	422
C_{4v}	$4 \cdot m$	$4mm$	$4mm$
D_{2d}	$\tilde{4} : 2$	$\bar{4}2m$ or $\bar{4}m2$	$\bar{4}2m$ or $\bar{4}m2$
D_{4h}	$m \cdot 4 : m$	$4/mmm$	$4/m\ 2/m\ 2/m$
C_3	3	3	3
C_{3i}	$\tilde{6}$	$\bar{3}$	$\bar{3}$
D_3	$3 : 2$	32 or 321 or 312	32 or 321 or 312
C_{3v}	$3 \cdot m$	$3m$ or $3m1$ or $31m$	$3m$ or $3m1$ or $31m$
D_{3d}	$\tilde{6} \cdot m$	$\bar{3}m$ or $\bar{3}m1$ or $\bar{3}1m$	$\bar{3}\ 2/m$ or $\bar{3}\ 2/m1$ or $\bar{3}12/m$
C_6	6	6	6
C_{3h}	$3 : m$	$\bar{6}$	$\bar{6}$
C_{6h}	$6 : m$	$6/m$	$6/m$
D_6	$6 : 2$	622	622
C_{6v}	$6 \cdot m$	$6mm$	$6mm$
D_{3h}	$m \cdot 3 : m$	$\bar{6}m2$ or $\bar{6}2m$	$\bar{6}m2$ or $\bar{6}2m$
D_{6h}	$m \cdot 6 : m$	$6/mmm$	$6/m\ 2/m\ 2/m$
T	$3/2$	23	23
T_h	$\tilde{6}/2$	$m\bar{3}$	$2/m\bar{3}$
O	$3/4$	432	432
T_d	$3/\tilde{4}$	$\bar{4}3m$	$\bar{4}3m$
O_h	$\tilde{6}/4$	$m\bar{3}m$	$4/m\ \bar{3}\ 2/m$

(i) components that represent the type of the generating operation, which are called *generators*;

(ii) components that are not used as generators but that serve to fix the directions of other symmetry elements (Hermann, 1931), and which are called *indicators*.

The generating matrices are uniquely defined by (i) and (ii) if it is assumed that they describe motions with counterclockwise rotational sense about the representative direction looked at end on by the observer. The symbols 2, 4, $\bar{4}$, 6 and $\bar{6}$ referring to direction [001] are indicators when the point-group symbol uses three sets of lattice symmetry directions. For instance, in 4*mm* the indicator 4 fixes the directions of the mirrors normal to [100] and [$1\bar{1}0$].

Note: The generation of (*a*) point group 432 by a rotation 3 around [111] and a rotation 2 and (*b*) point group $\bar{4}3m$ by 3 around [111] and a reflection *m* is only possible if the representative direction of the tertiary set is changed from [$1\bar{1}0$] to [110]; otherwise only the subgroup 32 or 3*m* of 432 or $\bar{4}3m$ will be generated.

3.3.2. Space-group symbols

3.3.2.1. Introduction

Each space group is related to a crystallographic point group. Space-group symbols, therefore, can be obtained by a modification of point-group symbols. The simplest modification which merely gives an enumeration of the space-group types (*cf.* Section 1.3.4.1) has been used by Schoenflies. The Shubnikov and Hermann–Mauguin symbols, however, reveal the glide or screw components of the symmetry operations and are designed in such a way that the nature of the symmetry elements and their relative locations can be deduced from the symbol. [A detailed discussion and listings of computer-adapted space-group symbols implemented in crystallographic software, such as the so-called *Hall symbols* (Hall, 1981*a*,*b*) or *explicit symbols* (Shmueli, 1984), can be found in Chapter 1.4 of *International Tables for Crystallography*, Volume B (2008).]

3.3.2.2. Schoenflies symbols

Space groups related to one point group are distinguished by adding a numerical superscript to the point-group symbol. Thus, the space groups related to the point group C_2 are called C_2^1, C_2^2, C_2^3.

3.3.2.3. The role of translation parts in the Shubnikov and Hermann–Mauguin symbols

A crystallographic symmetry operation W (*cf.* Chapter 1.2) is described by a pair of matrices

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{w})(\boldsymbol{W}, \boldsymbol{o}).$$

$\boldsymbol{W}$ is called the *rotation part*, $\boldsymbol{w}$ describes the *translation part* and determines the translation vector **w** of the operation. The translation part $\boldsymbol{w}$ can be decomposed into a *glide/screw part* $\boldsymbol{w}_g$ and a *location part* $\boldsymbol{w}_l$: $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$; here, $\boldsymbol{w}_l$ determines the location of the corresponding symmetry element with respect to the origin. The glide/screw part $\boldsymbol{w}_g$ may be derived by projecting $\boldsymbol{w}$ on the space invariant under $\boldsymbol{W}$, *i.e.* for rotations and reflections $\boldsymbol{w}$ is projected on the corresponding rotation axis or mirror plane. With matrix notation, $\boldsymbol{w}_g$ is determined by $(\boldsymbol{W}, \boldsymbol{w})^k = (\boldsymbol{I}, \boldsymbol{t})$ and $\boldsymbol{w}_g = (m/k)\boldsymbol{t}_1$, where k is the order of $\boldsymbol{W}$, the integers m are restricted by $0 \leq m < k$ and $\boldsymbol{t}_1$ is the shortest lattice vector in the direction of $\boldsymbol{t}$ (for details, *cf.* Sections 1.2.2.4 and 1.5.4.1). Space groups contain sets of screw and rotation axes or glide and mirror planes. A screw rotation is symbolized by k_m. The Shubnikov notation and the international notation use the same symbols for screw rotations. The symbols for glide reflections in both notations are listed in Table 3.3.2.1.

Table 3.3.2.1

Symbols of glide planes in the Shubnikov and Hermann–Mauguin space-group symbols

Glide plane perpendicular to	Glide vector	Shubnikov symbol	Hermann–Mauguin symbol
b or **c**	$\frac{1}{2}\mathbf{a}$	$\tilde{a}$	a
a or **c**	$\frac{1}{2}\mathbf{b}$	$\tilde{b}$	b
a or **b** or **a** − **b**	$\frac{1}{2}\mathbf{c}$	$\tilde{c}$	c
c	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\widetilde{ab}$	n
a	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$	$\widetilde{bc}$	n
b	$\frac{1}{2}(\mathbf{c}+\mathbf{a})$	$\widetilde{ac}$	n
a − **b**	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\widetilde{abc}$	n
c	$\frac{1}{4}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}\widetilde{ab}$	d
a	$\frac{1}{4}(\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{bc}$	d
b	$\frac{1}{4}(\mathbf{c}+\mathbf{a})$	$\frac{1}{2}\widetilde{ac}$	d
a − **b**	$\frac{1}{4}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{abc}$	d
a + **b**	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$		d

If the point-group symbol contains only one generator, the related space group is described completely by the Bravais lattice and a symbol corresponding to that of the point group in which rotations and reflections are replaced by screw rotations or glide reflections, if necessary. If, however, two or more operations generate the point group, it is necessary to have information on the mutual orientations and locations of the corresponding space-group symmetry elements, *i.e.* information on the location components $\boldsymbol{w}_l$. This is described in the following sections.

3.3.2.4. Shubnikov symbols

For the description of the mutual orientation of symmetry elements, the same symbols as for point groups are applied. In space groups, however, the symmetry elements need not intersect. In this case, the orientational symbols · (dot), : (colon), / (slash) are modified to $\odot$, $\textcircled{:}$, //. The space-group symbol starts with a description of the lattice defined by the basis **a**, **b**, **c**. For centred cells, the vectors to the centring points are given first. The same letters are used for basis vectors related by symmetry. The relative orientations of the vectors are denoted by the orientational symbols introduced above. The description of the lattice given in parentheses is followed by symbols of the generating elements of the related point group. If necessary, the symbols of the symmetry operations are modified to indicate their glide/screw parts. The first generator is separated from the lattice description by an orientation symbol. If this generator represents a mirror or glide plane, the dot connects the plane with the last two vectors whereas the colon refers only to the last vector. If the generator represents a rotation or a rotoreflection, the colon orients the related axis perpendicular to the plane given by the last two vectors whereas the dot refers only to the last vector. Two generators are separated by the symbols mentioned above to denote their relative orientations and sites. To make this description unique for space groups related to point group $O_h \equiv \tilde{6}/4$ with Bravais lattices *cP* and *cF*, it is necessary to use three generators instead of two: $4/\tilde{6} \cdot m$. For the sake of unification, this kind of description is extended to the remaining two space groups having Bravais lattice *cI*.

Example: Shubnikov symbol for the space group with Schoenflies symbol D_{2h}^{26} (72)

The Bravais lattice is *oI* (orthorhombic, body-centred). Therefore, the symbol for the lattice basis is

$$\left(\frac{a+b+c}{2}\Big/ c:(a:b)\right),$$

indicating that there is a centring vector $1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$ relative to the conventional orthorhombic cell. This vector is oblique with respect to the basis vector **c**, which is orthogonal to the perpendicular pair **a** and **b**. The basis vectors have independent lengths and are thus indicated by different letters *a*, *b* and *c* in arbitrary sequence.

To complete the symbol of the space group, we consider the point group D_{2h}. Its Shubnikov symbol is $m:2\cdot m$. Parallel to the (**a**, **b**) plane, there is a glide plane $\widetilde{ab}$ and a mirror plane *m*. The latter is chosen as generator. From the screw axis 2_1 and the rotation axis 2, both parallel to **c**, the latter is chosen as generator. The third generator can be a glide plane *c* perpendicular to **b**. Thus the Shubnikov symbol of D_{2h}^{26} is

$$\left(\frac{a+b+c}{2}\Big/ c:(a:b)\right)\cdot m:2\cdot\tilde{c}.$$

The list of all Shubnikov symbols is given in column 3 of Table 3.3.3.1.

3.3.2.5. International short symbols

The international symbol of a space group consists of two parts, just like the Shubnikov symbol. The first part is a capital letter that describes the type of centring of the conventional cell. It is followed by a modified point-group symbol that refers to the lattice symmetry directions. Centring type and point-group symbol determine the Bravais type of the translation group (*cf.* Section 3.1.1) and thus the point group of the lattice and the appropriate lattice symmetry directions. To derive the short international symbol of a given space group, the short symbol of the related point group must be modified in such a way that not only the rotation parts of the generating operations but also their translation parts can be constructed. This can be done by the following procedure:

(i) The glide/screw parts of generators and indicators are symbolized by applying the symbols for glide planes in Table 3.3.2.1 and the appropriate rules for screw rotations.

(ii) The generators are chosen in such a way that the related symmetry elements do intersect as far as possible. Exceptions may occur for space groups related to the pure rotation point groups 222, 422, 622, 23 and 432. In these cases, the axes of the generators may or may not intersect.

(iii) Subgroups of lattice point groups may have lattice symmetry directions with which no symmetry elements are associated. Such symmetry directions are symbolized by '1'. This symbol can only be omitted if no ambiguity arises, *e.g.* $P4/m11$ is reduced to $P4/m$. $P31m$ and $P3m1$, however, cannot be reduced. The use of the symbol '1' is discussed by Buerger (1967) and Donnay (1969, 1977).

Example

Again consider space group D_{2h}^{26} (72). The space group contains glide planes *c* and *b* perpendicular to the primary set, *c* and *a* normal to the secondary set of symmetry directions and *m* and *n* perpendicular to the tertiary set. To determine the short symbol, one generator must be chosen from each pair. The standardization rules (see the following section) lead to the symbol *Ibam*.

3.3.3. Properties of the international symbols

3.3.3.1. Derivation of the space group from the short symbol

Because the short international symbol contains a set of generators, it is possible to deduce the space group from it. With the same distinction between generators and indicators as for point groups, the modified point-group symbol directly gives the rotation parts $\boldsymbol{W}$ of the generating operations ($\boldsymbol{W}$, $\boldsymbol{w}$).

The modified symbols of the generators determine the glide/screw parts $\boldsymbol{w}_g$ of $\boldsymbol{w}$. To find the location parts $\boldsymbol{w}_l$ of $\boldsymbol{w}$, it is necessary to inspect the product relations of the group. The deduction of the set of complete generating operations can be summarized in the following rules:

(i) The integral translations are included in the set of generators. If the unit cell has centring points, the centring operations are generators.

(ii) The location parts of the generators can be set to zero except for the two cases noted under (iii) and (iv).

(iii) For non-cubic rotation groups with indicators in the symbol, the location part of the first generator can be set to zero. The location part of the second generator is $\boldsymbol{w}_l=\begin{pmatrix}0\\0\\-m/n\end{pmatrix}$; the intersection parameter $-m/n$ is derived from the indicator n_m in the [001] direction [*cf.* example (3) below].

(iv) For cubic rotation groups, the location part of the threefold rotation can be set to zero. For space groups related to the point group 23, the location part of the twofold rotation is $\boldsymbol{w}_l=\begin{pmatrix}-m/n\\0\\0\end{pmatrix}$ derived from the symbol n_m of the twofold operation itself. For space groups related to the point group 432, the location part of the twofold generating rotation is $\boldsymbol{w}_l=\begin{pmatrix}-m/n\\m/n\\m/n\end{pmatrix}$ derived from the indicator n_m in the [001] direction [*cf.* examples (4) and (5) below].

The origin that is selected by these rules is called the '*origin of the symbol*' (Burzlaff & Zimmermann, 1980). It is evident that the reference to the origin of the symbol allows a very short and unique notation of all desirable origins by appending the components of the origin of the symbol $\mathbf{q}=(q_1,q_2,q_3)$ to the short space-group symbol, thus yielding the so-called *expanded* Hermann–Mauguin symbol. The shift of origin can be performed easily, for only the translation parts have to be changed. The components of the transformed translation part can be obtained by [*cf.* Section 1.5.2.3 and equation (1.5.2.13)]

$$\boldsymbol{w}'=\boldsymbol{w}+(\boldsymbol{W}-\boldsymbol{I})\boldsymbol{q}.$$

Applications can be found in Burzlaff & Zimmermann (2002).

Examples: Deduction of the generating operations from the short symbol

Some examples for the use of these rules are now described in detail. It is convenient to describe the symmetry operation

($\boldsymbol{W}$, $\boldsymbol{w}$) by the corresponding coordinate triplets, *i.e.* using the so-called shorthand notation, *cf.* Section 1.2.2. The coordinate triplets can be interpreted as combinations of two constituents: the first one consists of the coordinates of a point in general position after the application of $\boldsymbol{W}$ on x, y, z, while the second corresponds to the translation part $\boldsymbol{w}$ of the symmetry operation. The coordinate triplets of the symmetry operations are tabulated as the *general position* in the space-group tables (in some cases a shift of origin is necessary). If preference is given to full matrix notation, Table 1.2.2.1 may be used. The following examples contain, besides the description of the symmetry operations, references to the numbering of the general positions in the space-group tables of this volume; *cf.* Sections 2.1.3.9 and 2.1.3.11. Centring translations are written after the numbers, if necessary.

(1) $Pccm = D_{2h}^3$ (49)

Besides the integral translations, the generators, as given in the symbol, are according to rule (ii):

glide reflection c_{100}: $\bar{x}, y, z+\frac{1}{2}$ (8)
glide reflection c_{010}: $x, \bar{y}, z+\frac{1}{2}$ (7)
reflection m_{001}: $x, y, \bar{z}$ (6).

No shift of origin is necessary. The expanded symbol is $Pccm\langle 000\rangle$.

(2) $Ibam = D_{2h}^{26}$ (72)

According to rule (i), the I centring is an additional generating translation. Thus, the generators are:

I centring: $x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$ $(1)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
glide reflection b_{100}: $\bar{x}, y+\frac{1}{2}, z$ (8)
glide reflection a_{010}: $x+\frac{1}{2}, \bar{y}, z$ (7)
reflection m_{001}: $x, y, \bar{z}$ (6).

To obtain the tabulated general position, a shift of origin by $(-\frac{1}{4},-\frac{1}{4},0)$ is necessary, the expanded symbol is $Ibam\langle -\frac{1}{4}-\frac{1}{4}0\rangle$.

(3) $P4_12_12 = D_4^4$ (92)

Apart from the translations, the generating elements are:

screw rotation 2_1 in [100]: $x+\frac{1}{2}, \bar{y}, \bar{z}$ (6)
rotation 2 in [$1\bar{1}0$]: $\bar{y}, \bar{x}, \bar{z}+\frac{1}{4}$ (8).

According to rule (iii), the location part of the first generator, referring to the secondary set of symmetry directions, is equal to zero. For the second generator, the screw part is equal to zero. The location part is $\boldsymbol{w}_l = \begin{pmatrix} 0 \\ 0 \\ -\frac{1}{4} \end{pmatrix}$. The expanded symbol $P4_12_12\langle\frac{1}{4}-\frac{1}{4}-\frac{3}{8}\rangle$ gives the tabulated setting.

(4) $P2_13 = T^4$ (198)

According to rule (iv), the generators are

rotation 3 in [111]: z, x, y (5)
screw rotation 2_1 in [001]: $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$ (2).

Following rule (iv), the location part of the threefold axis must be set to zero. The screw part of the twofold axis in [001] is $\begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$, the location part is $\boldsymbol{w}_l = \begin{pmatrix} -\frac{1}{2} \\ 0 \\ 0 \end{pmatrix} \equiv \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}$. No origin shift is necessary. The expanded symbol is $P2_13\langle 000\rangle$.

(5) $P4_132 = O^7$ (213)

Besides the integral translations, the generators given by the symbol are:

rotation 3 in [111]: z, x, y (5)
rotation 2 in [110]: $y-\frac{1}{4}, x+\frac{1}{4}, \bar{z}+\frac{1}{4}$ (13).

The screw part of the twofold axis is zero. According to rule (iv), the location part is $\boldsymbol{w}_l = \begin{pmatrix} -\frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix}$. No origin shift is necessary. The expanded symbol is $P4_132\langle 000\rangle$.

3.3.3.2. Derivation of the full symbol from the short symbol

If the geometrical point of view is again considered, it is possible to derive the full international symbol for a space group. This full symbol can be interpreted as consisting of symmetry elements. It can be generated from the short symbol with the aid of products between symmetry operations. It is possible, however, to derive the glide/screw parts of the elements in the full symbol directly from the glide/screw parts of the short symbol.

The product of operations corresponding to non-parallel glide or mirror planes generates a rotation or screw axis parallel to the intersection line. The screw part of the rotation is equal to the sum of the projections of the glide components of the planes on the axis. The angle between the planes determines the rotation part of the axis. For 90°, we obtain a twofold, for 60° a threefold, for 45° a fourfold and for 30° a sixfold axis.

Example: $Pbcn = D_{2h}^{14}$ (60)

The product of b and c generates a screw axis 2_1 in the z direction because the sum of the glide components in the z direction is $\frac{1}{2}$. The product of c and n generates a screw axis 2_1 in the x direction and the product between b and n produces a rotation axis 2 in the y direction because the y components for b and n add up to $1 \equiv 0$ modulo integers.

Thus, the full symbol is

$$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}.$$

In most cases, the full symbol is identical with the short symbol; differences between full and short symbols can only occur for space groups corresponding to lattice point groups (holohedries) and to the point group $m\bar{3}$. In all these cases, the short symbol is extended to the full symbol by adding the symbol for the maximal purely rotational subgroup. A special procedure is in use for monoclinic space groups. To indicate the choice of coordinate axes, the full symbol is treated like an orthorhombic symbol, in which the directions without symmetry are indicated by '1', *even though they do not correspond to lattice symmetry directions in the monoclinic case.*

3.3.3.3. Non-symbolized symmetry elements

Certain symmetry elements are not given explicitly in the full symbol because they can easily be derived. They are:

(i) Rotoinversion axes that are not used to indicate the lattice symmetry directions.

(ii) Rotation axes 2 included in the axes 4, $\bar{4}$ and 6 and rotation axes 3 included in the axes $\bar{3}$, 6 and $\bar{6}$.

(iii) Additional symmetry elements occurring in space groups with centred unit cells, *cf.* Sections 1.4.2.4 and 1.5.4.1. These types of operation can be deduced from the product of the centring translation $(\boldsymbol{I}, \boldsymbol{g})$ with a symmetry operation $(\boldsymbol{W}, \boldsymbol{w})$. The new symmetry operation $(\boldsymbol{W}, \boldsymbol{g}+\boldsymbol{w})$ again has $\boldsymbol{W}$ as rotation part but a different glide/screw part if the component of $\boldsymbol{g}$ parallel to the symmetry element corresponding to $\boldsymbol{W}$ is not a lattice vector; *cf.* Section 1.5.4.1.

Example

Space group $C2/c$ (15) has a twofold axis along **b** with screw part $\boldsymbol{w}_g = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$. The translational part of the centring operation is $\boldsymbol{g} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$.

An additional axis parallel to **b** thus has a translation part $\boldsymbol{g}+\boldsymbol{w}_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$. The component $\begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$ indicates a screw axis 2_1 in the b direction, whereas the component $\begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}$ indicates the location of this axis in $\frac{1}{4}, y, 0$. Similarly, it can be shown that glide plane c combined with the centring gives a glide plane n.

In the same way, in rhombohedral and cubic space groups, a rotation axis 3 is accompanied by screw axes 3_1 and 3_2. In space groups with centred unit cells, the location parts of different symmetry elements may coincide. In $I\bar{4}2m$, for example, the mirror plane m contains simultaneously a non-symbolized glide plane n. The same applies to all mirror planes in $Fmmm$.

(iv) Symmetry elements with diagonal orientation always occur with different types of glide/screw parts simultaneously. In space group $P\bar{4}2m$ (111) the translation vector along a can be decomposed as

$$\boldsymbol{w} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ 0 \end{pmatrix} = \boldsymbol{w}_g + \boldsymbol{w}_l.$$

The diagonal mirror plane with normal along $[1\bar{1}0]$ passing through the origin is accompanied by a parallel glide plane with glide part $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ passing through $\frac{1}{4}, -\frac{1}{4}, 0$. The same arguments lead to the occurrence of screw axes 2_1, 3_1 and 3_2 connected with diagonal rotation axes 2 or 3.

(v) For some investigations connected with *klassengleiche* subgroups (for subgroups of space groups, *cf.* Section 1.7.1), it is convenient to introduce an *extended Hermann–Mauguin symbol* that comprises all symmetry elements indicated in (iii) and (iv). The basic concept may be found in papers by Hermann (1929) and in *IT* (1952). These concepts have been applied by Bertaut (1976) and Zimmermann (1976); *cf.* Section 1.5.4.1.

Example

The full symbol of space group $Imma$ (74) is

$$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}.$$

The I-centring operation introduces additional rotation axes and glide planes for all three sets of lattice symmetry directions. The extended Hermann–Mauguin symbol is

$$I\frac{2,2_1}{m,n}\frac{2,2_1}{m,n}\frac{2,2_1}{a,b} \quad \text{or} \quad I\begin{matrix} \frac{2_1}{m} & \frac{2_1}{m} & \frac{2_1}{a} \\ \frac{2}{n} & \frac{2}{n} & \frac{2}{b} \end{matrix}.$$

This symbol shows immediately the eight subgroups with a P lattice corresponding to point group mmm:

$Pmma \sim Pmmb$, $Pnma \sim Pmnb$, $Pmna \sim Pnmb$ and $Pnna \sim Pnnb$.

3.3.3.4. Standardization rules for short symbols

The symbols of Bravais lattices and glide planes depend on the choice of basis vectors. As shown in the preceding section, additional translation vectors in centred unit cells produce new symmetry operations with the same rotation but different glide/screw parts. Moreover, it was shown that for diagonal orientations symmetry operations may be represented by different symbols. Thus, different short symbols for the same space group can be derived even if the rules for the selection of the generators and indicators are obeyed.

For the unique designation of a space-group type, a standardization of the short symbol is necessary. Rules for standardization were given first by Hermann (1931) and later in a slightly modified form in *IT* (1952).

These rules, which are generally followed in the present tables, are given below. Because of the historical development of the symbols (*cf.* Section 3.3.4), some of the present symbols do not obey the rules, whereas others depending on the crystal class need additional rules for them to be uniquely determined. These exceptions and additions are not explicitly mentioned, but may be discovered from Table 3.3.3.1 in which the short symbols are listed for all space groups. A table for all settings may be found in Section 1.5.4.

Triclinic symbols are unique if the unit cell is primitive. For the standard setting of *monoclinic* space groups, the lattice symmetry direction is labelled b. From the three possible centrings A, I and C, the latter one is favoured. If glide components occur in the plane perpendicular to [010], the glide direction c is preferred. In the space groups corresponding to the *orthorhombic* group $mm2$, the unique direction of the twofold axis is chosen along **c**. Accordingly, the face centring C is employed for centrings perpendicular to the privileged direction. For space groups with possible A or B centring, the first one is preferred. For groups 222 and mmm, no privileged symmetry direction exists, so the different possibilities of one-face centring can be reduced to C centring by change of the setting. The choices of unit cell and centring type are fixed by the conventional basis in systems with higher symmetry.

When more than one kind of symmetry elements exist in one representative direction, in most cases the choice for the space-group symbol is made in order of decreasing priority: for reflections and glide reflections m, a, b, c, n, d; for proper rotations and screw rotations 6, 6_1, 6_2, 6_3, 6_4, 6_5; 4, 4_1, 4_2, 4_3; 3, 3_1, 3_2; 2, 2_1 [*cf.* *IT* (1952), p. 55, and Section 1.4.1].

(*continued on page* 789)

Table 3.3.3.1
Standard space-group symbols

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*: 1935 Edition, Short	1935 Edition, Full	Present Edition, Short	Present Edition, Full	Comments†
1	C_1^1	$(a/b/c)\cdot 1$	$P1$	$P1$	$P1$	$P1$	
2	C_i^1	$(a/b/c)\cdot \tilde{2}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$(a/b/c)\cdot\bar{1}$ (Sh–K)
3	C_2^1	$(b:(c/a)):2$	$P2$	$P2$	$P2$	$P121$	
		$(c:(a/b)):2$				$P112$	
4	C_2^2	$(b:(c/a)):2_1$	$P2_1$	$P2_1$	$P2_1$	$P12_11$	
		$(c:(a/b)):2_1$				$P112_1$	
5	C_2^3	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right):2$	$C2$	$C2$	$C2$	$C121$	$B2$, $B112$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right):2$				$A112$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right):2$ (Sh–K)
6	C_s^1	$(b:(c/a))\cdot m$	Pm	Pm	Pm	$P1m1$	
		$(c:(a/b))\cdot m$				$P11m$	
7	C_s^2	$(b:(c/a))\cdot \tilde{c}$	Pc	Pc	Pc	$P1c1$	Pb, $P11b$ (*IT*, 1952)
		$(c:(b/a))\cdot \tilde{a}$				$P11a$	$(c:(a/b))\cdot\tilde{b}$ (Sh–K)
8	C_s^3	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right)\cdot m$	Cm	Cm	Cm	$C1m1$	Bm, $B11m$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right)\cdot m$				$A11m$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right)\cdot m$ (Sh–K)
9	C_s^4	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right)\cdot \tilde{c}$	Cc	Cc	Cc	$C1c1$	Bb, $B11b$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right)\cdot \tilde{a}$				$A11a$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right)\cdot\tilde{b}$ (Sh–K)
10	C_{2h}^1	$(b:(c/a))\cdot m:2$	$P2/m$	$P2/m$	$P2/m$	$P1\ 2/m1$	
		$(c:(a/b))\cdot m:2$				$P11\ 2/m$	
11	C_{2h}^2	$(b:(c/a))\cdot m:2_1$	$P2_1/m$	$P2_1/m$	$P2_1/m$	$P1\ 2_1/m\ 1$	
		$(c:(a/b))\cdot m:2_1$				$P11\ 2_1/m$	
12	C_{2h}^3	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right)\cdot m:2$	$C2/m$	$C2/m$	$C2/m$	$C1\ 2/m\ 1$	$B2/m$, $B11\ 2/m$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right)\cdot m:2$				$A11\ 2/m$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right)\cdot m:2$ (Sh–K)
13	C_{2h}^4	$(b:(c/a))\cdot \tilde{c}:2$	$P2/c$	$P2/c$	$P2/c$	$P1\ 2/c\ 1$	$P2/b$, $P11\ 2/b$ (*IT*, 1952)
		$(c:(a/b))\cdot \tilde{a}:2$				$P11\ 2/a$	$(c:(a/b))\cdot\tilde{b}:2$ (Sh–K)
14	C_{2h}^5	$(b:(c/a))\cdot \tilde{c}:2_1$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P1\ 2_1/c\ 1$	$P2_1/b$, $P112_1/b$ (*IT*, 1952)
		$(c:(a/b))\cdot \tilde{a}:2_1$				$P11\ 2_1/a$	$(c:(a/b))\cdot b:2_1$ (Sh–K)
15	C_{2h}^6	$\left(\frac{a+b}{2}\Big/ b:(c/a)\right)\cdot \tilde{c}:2$	$C2/c$	$C2/c$	$C2/c$	$C1\ 2/c\ 1$	$B2/b$, $B11\ 2/b$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\Big/ c:(b/a)\right)\cdot \tilde{a}:2$				$A11\ 2a$	$\left(\frac{a+c}{2}\Big/ c:(a/b)\right)\cdot\tilde{b}:2$ (Sh–K)
16	D_2^1	$(c:(a:b)):2:2$	$P222$	$P222$	$P222$	$P222$	
17	D_2^2	$(c:(a:b)):2_1:2$	$P222_1$	$P222_1$	$P222_1$	$P222_1$	
18	D_2^3	$(c:(a:b)):2\odot 2_1$	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P2_12_12$	
19	D_2^4	$(c:(a:b)):2_1\odot 2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	
20	D_2^5	$\left(\frac{a+b}{2}:c:(a:b)\right):2_1:2$	$C222_1$	$C222_1$	$C222_1$	$C222_1$	
21	D_2^6	$\left(\frac{a+b}{2}:c:(a:b)\right):2:2$	$C222$	$C222$	$C222$	$C222$	
22	D_2^7	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right):2:2$	$F222$	$F222$	$F222$	$F222$	
23	D_2^8	$\left(\frac{a+b+c}{2}\Big/ c:(a:b)\right):2:2$	$I222$	$I222$	$I222$	$I222$	
24	D_2^9	$\left(\frac{a+b+c}{2}\Big/ c:(a:b)\right):2:2_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	
25	C_{2v}^1	$(c:(a:b)):m\cdot 2$	Pmm	$Pmm2$	$Pmm2$	$Pmm2$	
26	C_{2v}^2	$(c:(a:b)):\tilde{c}\cdot 2_1$	Pmc	$Pmc2_1$	$Pmc2_1$	$Pmc2_1$	
27	C_{2v}^3	$(c:(a:b)):\tilde{c}\cdot 2$	Pcc	$Pcc2$	$Pcc2$	$Pcc2$	

Table 3.3.3.1 (continued)

No.	Schoen-flies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
28	C_{2v}^{4}	$(c:(a:b)):\tilde{a}\cdot 2$	Pma	$Pma2$	$Pma2$	$Pma2$	
29	C_{2v}^{5}	$(c:(a:b)):\tilde{a}\cdot 2_1$	Pca	$Pca2_1$	$Pca2_1$	$Pca2_1$	
30	C_{2v}^{6}	$(c:(a:b)):\tilde{c}\odot 2$	Pnc	$Pnc2$	$Pnc2$	$Pnc2$	$(c:(a:b)):\widetilde{ac}\cdot 2$ (Sh–K)
31	C_{2v}^{7}	$(c:(a:b)):\widetilde{ac}\cdot 2_1$	Pmn	$Pmn2_1$	$Pmn2_1$	$Pmn2_1$	
32	C_{2v}^{8}	$(c:(a:b)):\tilde{a}\odot 2$	Pba	$Pba2$	$Pba2$	$Pba2$	
33	C_{2v}^{9}	$(c:(a:b)):\tilde{a}\odot 2_1$	Pna	$Pna2_1$	$Pna2_1$	$Pna2_1$	
34	C_{2v}^{10}	$(c:(a:b)):\widetilde{ac}\odot 2$	Pnn	$Pnn2$	$Pnn2$	$Pnn2$	
35	C_{2v}^{11}	$\left(\frac{a+b}{2}:c:(a:b)\right):m\cdot 2$	Cmm	$Cmm2$	$Cmm2$	$Cmm2$	
36	C_{2v}^{12}	$\left(\frac{a+b}{2}:c:(a:b)\right):\tilde{c}\cdot 2_1$	Cmc	$Cmc2_1$	$Cmc2_1$	$Cmc2_1$	
37	C_{2v}^{13}	$\left(\frac{a+b}{2}:c:(a:b)\right):\tilde{c}\cdot 2$	Ccc	$Ccc2$	$Ccc2$	$Ccc2$	
38	C_{2v}^{14}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):m\cdot 2$	Amm	$Amm2$	$Amm2$	$Amm2$	
39	C_{2v}^{15}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):m\cdot 2_1$	Abm	$Abm2$	$Aem2$	$Aem2$	$\left(\frac{b+c}{2}/c:(a:b)\right):\tilde{c}\cdot 2$ (Sh–K) Use former symbol $Abm2$ for generation
40	C_{2v}^{16}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2$	Ama	$Ama2$	$Ama2$	$Ama2$	
41	C_{2v}^{17}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2_1$	Aba	$Aba2$	$Aea2$	$Aea2$	$\left(\frac{b+c}{2}/c:(a:b)\right):\widetilde{ac}\cdot 2$ (Sh–K) Use former symbol $Aba2$ for generation
42	C_{2v}^{18}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right):m\cdot 2$	Fmm	$Fmm2$	$Fmm2$	$Fmm2$	
43	C_{2v}^{19}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:\tilde{c}:(a:b)\right):\frac{1}{2}\widetilde{ac}\odot 2$	Fdd	$Fdd2$	$Fdd2$	$Fdd2$	
44	C_{2v}^{20}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):m\cdot 2$	Imm	$Imm2$	$Imm2$	$Imm2$	
45	C_{2v}^{21}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):\tilde{c}\cdot 2$	Iba	$Iba2$	$Iba2$	$Iba2$	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2_1$ (Sh–K)
46	C_{2v}^{22}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2$	Ima	$Ima2$	$Ima2$	$Ima2$	
47	D_{2h}^{1}	$(c:(a:b))\cdot m:2\cdot m$	$Pmmm$	$P2/m\ 2/m\ 2/m$	$Pmmm$	$P2/m\ 2/m\ 2/m$	
48	D_{2h}^{2}	$(c:(a:b))\cdot\widetilde{ab}:2\odot\widetilde{ac}$	$Pnnn$	$P2/n\ 2/n\ 2/n$	$Pnnn$	$P2/n\ 2/n\ 2/n$	
49	D_{2h}^{3}	$(c:(a:b))\cdot m:2\cdot\tilde{c}$	$Pccm$	$P2/c\ 2/c\ 2/m$	$Pccm$	$P2/c\ 2/c\ 2/m$	
50	D_{2h}^{4}	$(c:(a:b))\cdot\widetilde{ab}:2\odot\tilde{a}$	$Pban$	$P2/b\ 2/a\ 2/n$	$Pban$	$P2/b\ 2/a\ 2/n$	
51	D_{2h}^{5}	$(c:(a:b))\cdot\tilde{a}:2\cdot m$	$Pmma$	$P2_1/m\ 2/m\ 2/a$	$Pmma$	$P2_1/m\ 2/m\ 2/a$	
52	D_{2h}^{6}	$(c:(a:b))\cdot\tilde{a}:2\odot\widetilde{ac}$	$Pnna$	$P2/n\ 2_1/n\ 2/a$	$Pnna$	$P2/n\ 2_1/n\ 2/a$	
53	D_{2h}^{7}	$(c:(a:b))\cdot\tilde{a}:2_1\cdot\widetilde{ac}$	$Pmna$	$P2/m\ 2/n\ 2_1/a$	$Pmna$	$P2/m\ 2/n\ 2_1/a$	
54	D_{2h}^{8}	$(c:(a:b))\cdot\tilde{a}:2\cdot\tilde{c}$	$Pcca$	$P2_1/c\ 2/c\ 2/a$	$Pcca$	$P2_1/c\ 2/c\ 2/a$	
55	D_{2h}^{9}	$(c:(a:b))\cdot m:2\odot\tilde{a}$	$Pbam$	$P2_1/b\ 2_1/a\ 2/m$	$Pbam$	$P2_1/b\ 2_1/a\ 2/m$	
56	D_{2h}^{10}	$(c:(a:b))\cdot\widetilde{ab}:2\cdot\tilde{c}$	$Pccn$	$P2_1/c\ 2_1/c\ 2/n$	$Pccn$	$P2_1/c\ 2_1/c\ 2/n$	
57	D_{2h}^{11}	$(c:(a:b))\cdot m:2_1\odot\tilde{c}$	$Pbcm$	$P2/b\ 2_1/c\ 2_1/m$	$Pbcm$	$P2/b\ 2_1/c\ 2_1/m$	
58	D_{2h}^{12}	$(c:(a:b))\cdot m:2\odot\widetilde{ac}$	$Pnnm$	$P2_1/n\ 2_1/n\ 2/m$	$Pnnm$	$P2_1/n\ 2_1/n\ 2/m$	
59	D_{2h}^{13}	$(c:(a:b))\cdot\widetilde{ab}:2\cdot m$	$Pmmn$	$P2_1/m\ 2_1/m\ 2/n$	$Pmmn$	$P2_1/m\ 2_1/m\ 2/n$	
60	D_{2h}^{14}	$(c:(a:b))\cdot\widetilde{ab}:2_1\odot\tilde{c}$	$Pbcn$	$P2_1/b\ 2/c\ 2_1/n$	$Pbcn$	$P2_1/b\ 2/c\ 2_1/n$	
61	D_{2h}^{15}	$(c:(a:b))\cdot\tilde{a}:2_1\odot\tilde{c}$	$Pbca$	$P2_1/b\ 2_1/c\ 2_1/a$	$Pbca$	$P2_1/b\ 2_1/c\ 2_1/a$	
62	D_{2h}^{16}	$(c:(a:b))\cdot\tilde{a}:2_1\odot m$	$Pnma$	$P2_1/n\ 2_1/m\ 2_1/a$	$Pnma$	$P2_1/n\ 2_1/m\ 2_1/a$	
63	D_{2h}^{17}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot m:2_1\cdot\tilde{c}$	$Cmcm$	$C2/m\ 2/c\ 2_1/m$	$Cmcm$	$C2/m\ 2/c\ 2_1/m$	
64	D_{2h}^{18}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot\tilde{a}:2_1\cdot\tilde{c}$	$Cmca$	$C2/m\ 2/c\ 2_1/a$	$Cmce$	$C2/m\ 2/c\ 2_1/e$	Use former symbol $Cmca$ for generation

Table 3.3.3.1 (continued)

No.	Schoen-flies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
65	D_{2h}^{19}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot m:2\cdot m$	*Cmmm*	$C2/m\ 2/m\ 2/m$	*Cmmm*	$C2/m\ 2/m\ 2/m$	
66	D_{2h}^{20}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot m:2\cdot \tilde{c}$	*Cccm*	$C2/c\ 2/c\ 2/m$	*Cccm*	$C2/c\ 2/c\ 2/m$	
67	D_{2h}^{21}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot \tilde{a}:2\cdot m$	*Cmma*	$C2/m\ 2/m\ 2/a$	*Cmme*	$C2/m\ 2/m\ 2/e$	Use former symbol *Cmma* for generation
68	D_{2h}^{22}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot \tilde{a}:2\cdot \tilde{c}$	*Ccca*	$C2/c\ 2/c\ 2/a$	*Ccce*	$C2/c\ 2/c\ 2/e$	Use former symbol *Ccca* for generation
69	D_{2h}^{23}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right)$ $\cdot m:2\cdot m$	*Fmmm*	$F2/m\ 2/m\ 2/m$	*Fmmm*	$F2/m\ 2/m\ 2/m$	
70	D_{2h}^{24}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right)$ $\cdot\frac{1}{2}\widetilde{ab}:2\odot\frac{1}{2}\widetilde{ac}$	*Fddd*	$F2/d\ 2/d\ 2/d$	*Fddd*	$F2/d\ 2/d\ 2/d$	
71	D_{2h}^{25}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot m:2\cdot m$	*Immm*	$I2/m\ 2/m\ 2/m$	*Immm*	$I2/m\ 2/m\ 2/m$	
72	D_{2h}^{26}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot m:2\cdot \tilde{c}$	*Ibam*	$I2/b\ 2/a\ 2/m$	*Ibam*	$I2/b\ 2/a\ 2/m$	
73	D_{2h}^{27}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot \tilde{a}:2\cdot \tilde{c}$	*Ibca*	$I2_1/b\ 2_1/c\ 2_1/a$	*Ibca*	$I2_1/b\ 2_1/c\ 2_1/a$	$I2/b\ 2/c\ 2/a$ (*IT*, 1952)
74	D_{2h}^{28}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right)\cdot \tilde{a}:2\cdot m$	*Imma*	$I2_1/m\ 2_1/m\ 2_1/a$	*Imma*	$I2_1/m\ 2_1/m\ 2_1/a$	$I2/m\ 2/m\ 2/a$ (*IT*, 1952)
75	C_4^1	$(c:(a:a)):4$	$P4$	$P4$	$P4$	$P4$	
76	C_4^2	$(c:(a:a)):4_1$	$P4_1$	$P4_1$	$P4_1$	$P4_1$	
77	C_4^3	$(c:(a:a)):4_2$	$P4_2$	$P4_2$	$P4_2$	$P4_2$	
78	C_4^4	$(c:(a:a)):4_3$	$P4_3$	$P4_3$	$P4_3$	$P4_3$	
79	C_4^5	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4$	$I4$	$I4$	$I4$	$I4$	
80	C_4^6	$\left(\frac{a-b-c}{2}\Big/c:(a:a)\right):4_1$	$I4_1$	$I4_1$	$I4_1$	$I4_1$	
81	S_4^1	$(c:(a:a)):\tilde{4}$	$P\bar{4}$	$P\bar{4}$	$P\bar{4}$	$P\bar{4}$	
82	S_4^2	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):\tilde{4}$	$I\bar{4}$	$I\bar{4}$	$I\bar{4}$	$I\bar{4}$	
83	C_{4h}^1	$(c:(a:a))\cdot m:4$	$P4/m$	$P4/m$	$P4/m$	$P4/m$	
84	C_{4h}^2	$(c:(a:a))\cdot m:4_2$	$P4_2/m$	$P4_2/m$	$P4_2/m$	$P4_2/m$	
85	C_{4h}^3	$(c:(a:a))\cdot \widetilde{ab}:4$	$P4/n$	$P4/n$	$P4/n$	$P4/n$	
86	C_{4h}^4	$(c:(a:a))\cdot \widetilde{ab}:4_2$	$P4_2/n$	$P4_2/n$	$P4_2/n$	$P4_2/n$	
87	C_{4h}^5	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot m:4$	$I4/m$	$I4/m$	$I4/m$	$I4/m$	
88	C_{4h}^6	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot \tilde{a}:4_1$	$I4_1/a$	$I4_1/a$	$I4_1/a$	$I4_1/a$	
89	D_4^1	$(c:(a:a)):4:2$	$P42$	$P422$	$P422$	$P422$	
90	D_4^2	$(c:(a:a)):4\odot 2_1$	$P42_1$	$P42_12$	$P42_12$	$P42_12$	
91	D_4^3	$(c:(a:a)):4_1:2$	$P4_12$	$P4_122$	$P4_122$	$P4_122$	
92	D_4^4	$(c:(a:a)):4_1\odot 2_1$	$P4_12_1$	$P4_12_12$	$P4_12_12$	$P4_12_12$	
93	D_4^5	$(c:(a:a)):4_2:2$	$P4_22$	$P4_222$	$P4_222$	$P4_222$	
94	D_4^6	$(c:(a:a)):4_2\odot 2_1$	$P4_22_1$	$P4_22_12$	$P4_22_12$	$P4_22_12$	
95	D_4^7	$(c:(a:a)):4_3:2$	$P4_32$	$P4_322$	$P4_322$	$P4_322$	
96	D_4^8	$(c:(a:a)):4_3\odot 2_1$	$P4_32_1$	$P4_32_12$	$P4_32_12$	$P4_32_12$	
97	D_4^9	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4:2$	$I42$	$I422$	$I422$	$I422$	
98	D_4^{10}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4_1:2$	$I4_12$	$I4_122$	$I4_122$	$I4_122$	
99	C_{4v}^1	$(c:(a:a)):4\cdot m$	*P4mm*	*P4mm*	*P4mm*	*P4mm*	
100	C_{4v}^2	$(c:(a:a)):4\odot \tilde{a}$	*P4bm*	*P4bm*	*P4bm*	*P4bm*	
101	C_{4v}^3	$(c:(a:a)):4_2\cdot \tilde{c}$	*P4cm*	$P4_2cm$	$P4_2cm$	$P4_2cm$	
102	C_{4v}^4	$(c:(a:a)):4_2\odot \widetilde{ac}$	*P4nm*	$P4_2nm$	$P4_2nm$	$P4_2nm$	

Table 3.3.3.1 (continued)

No.	Schoen-flies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
103	C_{4v}^{5}	$(c:(a:a)):4\cdot\tilde{c}$	$P4cc$	$P4cc$	$P4cc$	$P4cc$	
104	C_{4v}^{6}	$(c:(a:a)):4\odot\widetilde{ac}$	$P4nc$	$P4nc$	$P4nc$	$P4nc$	
105	C_{4v}^{7}	$(c:(a:a)):4_2\cdot m$	$P4mc$	$P4_2mc$	$P4_2mc$	$P4_2mc$	
106	C_{4v}^{8}	$(c:(a:a)):4_2\odot\tilde{a}$	$P4bc$	$P4_2bc$	$P4_2bc$	$P4_2bc$	
107	C_{4v}^{9}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4\cdot m$	$I4mm$	$I4mm$	$I4mm$	$I4mm$	
108	C_{4v}^{10}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4\cdot\tilde{c}$	$I4cm$	$I4cm$	$I4cm$	$I4cm$	
109	C_{4v}^{11}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4_1\odot m$	$I4md$	$I4_1md$	$I4_1md$	$I4_1md$	
110	C_{4v}^{12}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):4_1\odot\tilde{c}$	$I4cd$	$I4_1cd$	$I4_1cd$	$I4_1cd$	$\left(\frac{a+b+c}{2}\Big/c:a:a\right):4_1\cdot\tilde{a}$ (Sh–K)
111	D_{2d}^{1}	$(c:(a:a)):\tilde{4}:2$	$P\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2m$	
112	D_{2d}^{2}	$(c:(a:a)):\tilde{4}\odot 2$	$P\bar{4}2c$	$P\bar{4}2c$	$P\bar{4}2c$	$P\bar{4}2c$	
113	D_{2d}^{3}	$(c:(a:a)):\tilde{4}\cdot\widetilde{ab}$	$P\bar{4}2_1m$	$P\bar{4}2_1m$	$P\bar{4}2_1m$	$P\bar{4}2_1m$	
114	D_{2d}^{4}	$(c:(a:a)):\tilde{4}\cdot\widetilde{abc}$	$P\bar{4}2_1c$	$P\bar{4}2_1c$	$P\bar{4}2_1c$	$P\bar{4}2_1c$	
115	D_{2d}^{5}	$(c:(a:a)):\tilde{4}\cdot m$	$C\bar{4}2m$	$C\bar{4}2m$	$P\bar{4}m2$	$P\bar{4}m2$	
116	D_{2d}^{6}	$(c:(a:a)):\tilde{4}\cdot\tilde{c}$	$C\bar{4}2c$	$C\bar{4}2c$	$P\bar{4}c2$	$P\bar{4}c2$	
117	D_{2d}^{7}	$(c:(a:a)):\tilde{4}\odot\tilde{a}$	$C\bar{4}2b$	$C\bar{4}2b$	$P\bar{4}b2$	$P\bar{4}b2$	
118	D_{2d}^{8}	$(c:(a:a)):\tilde{4}\cdot\widetilde{ac}$	$C\bar{4}2n$	$C\bar{4}2n$	$P\bar{4}n2$	$P\bar{4}n2$	
119	D_{2d}^{9}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):\tilde{4}\cdot m$	$F\bar{4}2m$	$F\bar{4}2m$	$I\bar{4}m2$	$I\bar{4}m2$	
120	D_{2d}^{10}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):\tilde{4}\cdot\tilde{c}$	$F\bar{4}2c$	$F\bar{4}2c$	$I\bar{4}c2$	$I\bar{4}c2$	
121	D_{2d}^{11}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):\tilde{4}:2$	$I\bar{4}2m$	$I\bar{4}2m$	$I\bar{4}2m$	$I\bar{4}2m$	
122	D_{2d}^{12}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right):\tilde{4}\odot\frac{1}{2}\widetilde{abc}$	$I\bar{4}2d$	$I\bar{4}2d$	$I\bar{4}2d$	$I\bar{4}2d$	
123	D_{4h}^{1}	$(c:(a:a))\cdot m:4\cdot m$	$P4/mmm$	$P4/m\ 2/m\ 2/m$	$P4/mmm$	$P4/m\ 2/m\ 2/m$	
124	D_{4h}^{2}	$(c:(a:a))\cdot m:4\cdot\tilde{c}$	$P4/mcc$	$P4/m\ 2/c\ 2/c$	$P4/mcc$	$P4/m\ 2/c\ 2/c$	
125	D_{4h}^{3}	$(c:(a:a))\cdot\widetilde{ab}:4\odot\tilde{a}$	$P4/nbm$	$P4/n\ 2/b\ 2/m$	$P4/nbm$	$P4/n\ 2/b\ 2/m$	$(c:a:a)\cdot\widetilde{ab}:4\odot\tilde{b}$ (Sh–K)
126	D_{4h}^{4}	$(c:(a:a))\cdot\widetilde{ab}:4\odot\widetilde{ac}$	$P4/nnc$	$P4/n\ 2/n\ 2/c$	$P4/nnc$	$P4/n\ 2/n\ 2/c$	
127	D_{4h}^{5}	$(c:(a:a))\cdot m:4\odot\tilde{a}$	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$	$(c:a:a)\cdot m:4\odot\tilde{b}$ (Sh–K)
128	D_{4h}^{6}	$(c:(a:a))\cdot m:4\odot\widetilde{ac}$	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$	
129	D_{4h}^{7}	$(c:(a:a))\cdot\widetilde{ab}:4\cdot m$	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$	
130	D_{4h}^{8}	$(c:(a:a)\cdot\widetilde{ab}:4\cdot\tilde{c}$	$P4/ncc$	$P4/n\ 2/c\ 2/c$	$P4/ncc$	$P4/n\ 2/c\ 2/c$	
131	D_{4h}^{9}	$(c:(a:a))\cdot m:4_2\cdot m$	$P4/mmc$	$P4_2/m\ 2/m\ 2/c$	$P4_2/mmc$	$P4_2/m\ 2/m\ 2/c$	
132	D_{4h}^{10}	$(c:(a:a))\cdot m:4_2\cdot\tilde{c}$	$P4/mcm$	$P4_2/m\ 2/c\ 2/m$	$P4_2/mcm$	$P4_2/m\ 2/c\ 2/m$	
133	D_{4h}^{11}	$(c:(a:a))\cdot\widetilde{ab}:4_2\odot\tilde{a}$	$P4/nbc$	$P4_2/n\ 2/b\ 2/c$	$P4_2/nbc$	$P4_2/n\ 2/b\ 2/c$	$(c:a:a)\cdot\widetilde{ab}:4_2\odot\tilde{b}$ (Sh–K)
134	D_{4h}^{12}	$(c:(a:a))\cdot\widetilde{ab}:4_2\odot\widetilde{ac}$	$P4/nnm$	$P4_2/n\ 2/n\ 2/m$	$P4_2/nnm$	$P4_2/n\ 2/n\ 2/m$	
135	D_{4h}^{13}	$(c:(a:a))\cdot n:4_2\odot\tilde{a}$	$P4/mbc$	$P4_2/m\ 2_1/b\ 2/c$	$P4_2/mbc$	$P4_2/m\ 2_1/b\ 2/c$	$(c:a:a)\cdot m:4_2\odot\tilde{b}$ (Sh–K)
136	D_{4h}^{14}	$(c:(a:a))\cdot m:4_2\odot\widetilde{ac}$	$P4/mnm$	$P4_2/m\ 2_1/n\ 2/m$	$P4_2/mnm$	$P4_2/m\ 2_1/n\ 2/m$	
137	D_{4h}^{15}	$(c:(a:a))\cdot\widetilde{ab}:4_2\cdot m$	$P4/nmc$	$P4_2/n\ 2_1/m\ 2/c$	$P4_2/nmc$	$P4_2/n\ 2_1/m\ 2/c$	
138	D_{4h}^{16}	$(c:(a:a))\cdot ab:4_2\cdot\tilde{c}$	$P4/ncm$	$P4_2/n\ 2_1/c\ 2/m$	$P4_2/ncm$	$P4_2/n\ 2_1/c\ 2/m$	
139	D_{4h}^{17}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot m:4\cdot m$	$I4/mmm$	$I4/m\ 2/m\ 2/m$	$I4/mmm$	$I4/m\ 2/m\ 2/m$	
140	D_{4h}^{18}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot m:4\cdot\tilde{c}$	$I4/mcm$	$I4/m\ 2/c\ 2/m$	$I4/mcm$	$I4/m\ 2/c\ 2/m$	
141	D_{4h}^{19}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot\tilde{a}:4_1\odot m$	$I4/amd$	$I4_1/a\ 2/m\ 2/d$	$I4_1/amd$	$I4_1/a\ 2/m\ 2/d$	
142	D_{4h}^{20}	$\left(\frac{a+b+c}{2}\Big/c:(a:a)\right)\cdot\tilde{a}:4_1\odot\tilde{c}$	$I4/acd$	$I4_1/a\ 2/c\ 2/d$	$I4_1/acd$	$I4_1/a\ 2/c\ 2/d$	
143	C_{3}^{1}	$(c:(a/a)):3$	$C3$	$C3$	$P3$	$P3$	
144	C_{3}^{2}	$(c:(a/a)):3_1$	$C3_1$	$C3_1$	$P3_1$	$P3_1$	
145	C_{3}^{3}	$(c:(a/a)):3_2$	$C3_2$	$C3_2$	$P3_2$	$P3_2$	

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*: 1935 Edition, Short	1935 Edition, Full	Present Edition, Short	Present Edition, Full	Comments†
146	C_3^4	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):3$	$R3$	$R3$	$R3$	$R3$	Hexagonal setting (Sh–K)
		$(a/a/a)/3$					Rhombohedral setting (Sh–K)
147	C_{3i}^1	$(c:(a/a)):\tilde{6}$	$C\bar{3}$	$C\bar{3}$	$P\bar{3}$	$P\bar{3}$	
148	C_{3i}^2	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):\tilde{6}$	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6}$					Rhombohedral setting (Sh–K)
149	D_3^1	$(c:(a/a)):2:3$	$H32$	$H321$	$P312$	$P312$	
150	D_3^2	$(c:(a/a)):2:3$	$C32$	$C321$	$P321$	$P321$	
151	D_3^3	$(c:(a/a)):2:3_1$	$H3_12$	$H3_121$	$P3_112$	$P3_112$	
152	D_3^4	$(c:(a/a)):2:3_1$	$C3_12$	$C3_121$	$P3_121$	$P3_121$	
153	D_3^5	$(c:(a/a)):2:3_2$	$H3_22$	$H3_221$	$P3_212$	$P3_212$	
154	D_3^6	$(c:(a/a)):2:3_2$	$C3_22$	$C3_221$	$P3_221$	$P3_221$	
155	D_3^7	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right)\cdot 2:3$	$R32$	$R32$	$R32$	$R32$	Hexagonal setting (Sh–K)
		$(a/a/a)/3:2$					Rhombohedral setting (Sh–K)
156	C_{3v}^1	$(c:(a/a)):m:3$	$C3m$	$C3m1$	$P3m1$	$P3m1$	
157	C_{3v}^2	$(a:c:a):m:3$	$H3m$	$H3m1$	$P31m$	$P31m$	$(c:(a/a))\cdot m\cdot 3$ (Sh–K) with special comment
158	C_{3v}^3	$(c:(a/a)):\tilde{c}:3$	$C3c$	$C3c1$	$P3c1$	$P3c1$	
159	C_{3v}^4	$(a:c:a):\tilde{c}:3$	$H3c$	$H3c1$	$P31c$	$P31c$	$(c:(a/a))\cdot \tilde{c}\cdot 3$ (Sh–K) with special comment
160	C_{3v}^5	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right)\cdot m\cdot 3$	$R3m$	$R3m$	$R3m$	$R3m$	Hexagonal setting (Sh–K)
		$(a/a/a)/3\cdot m$					Rhombohedral setting (Sh–K)
161	C_{3v}^6	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right)\cdot \tilde{c}\cdot 3$	$R3c$	$R3c$	$R3c$	$R3c$	Hexagonal setting (Sh–K)
		$(a/a/a)/3\cdot\widetilde{abc}$					Rhombohedral setting (Sh–K)
162	D_{3d}^1	$(a:c:a)\cdot m\cdot\tilde{6}$	$H\bar{3}m$	$H\bar{3}\ 2/m\ 1$	$P\bar{3}1m$	$P\bar{3}1\ 2/m$	$(c:(a/a))\cdot m\cdot\tilde{6}$ (Sh–K) with special comment
163	D_{3d}^2	$(a:c:a)\cdot\tilde{c}\cdot\tilde{6}$	$H\bar{3}c$	$H\bar{3}\ 2/c\ 1$	$P\bar{3}1c$	$P\bar{3}1\ 2/c$	$(c:(a/a)\cdot\tilde{c}\cdot\tilde{6}$ (Sh–K) with special comment
164	D_{3d}^3	$(c:(a/a)):m\cdot\tilde{6}$	$C\bar{3}m$	$C\bar{3}\ 2/m\ 1$	$P\bar{3}m1$	$P\bar{3}\ 2/m\ 1$	
165	D_{3d}^4	$(c:(a/a)):\tilde{c}\cdot\tilde{6}$	$C\bar{3}c$	$C\bar{3}\ 2/c\ 1$	$P\bar{3}c1$	$P\bar{3}\ 2/c\ 1$	
166	D_{3d}^5	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):m\cdot\tilde{6}$	$R\bar{3}m$	$R\bar{3}\ 2/m$	$R\bar{3}m$	$R\bar{3}\ 2/m$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6}\cdot m$					Rhombohedral setting (Sh–K)
167	D_{3d}^6	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c:(a/a)\right):\tilde{c}\cdot\tilde{6}$	$R\bar{3}c$	$R\bar{3}\ 2/c$	$R\bar{3}c$	$R\bar{3}\ 2/c$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6}\cdot\widetilde{abc}$					Rhombohedral setting (Sh–K)
168	C_6^1	$(c:(a/a)):6$	$C6$	$C6$	$P6$	$P6$	
169	C_6^2	$(c:(a/a)):6_1$	$C6_1$	$C6_1$	$P6_1$	$P6_1$	
170	C_6^3	$(c:(a/a)):6_5$	$C6_5$	$C6_5$	$P6_5$	$P6_5$	
171	C_6^4	$(c:(a/a)):6_2$	$C6_2$	$C6_2$	$P6_2$	$P6_2$	
172	C_6^5	$(c:(a/a)):6_4$	$C6_4$	$C6_4$	$P6_4$	$P6_4$	
173	C_6^6	$(c:(a/a)):6_3$	$C6_3$	$C6_3$	$P6_3$	$P6_3$	
174	C_{3h}^1	$(c:(a/a)):3:m$	$C\bar{6}$	$C\bar{6}$	$P\bar{6}$	$P\bar{6}$	
175	C_{6h}^1	$(c:(a/a))\cdot m:6$	$C6/m$	$C6/m$	$P6/m$	$P6/m$	
176	C_{6h}^2	$(c:(a/a))\cdot m:6_3$	$C6_3/m$	$C6_3/m$	$P6_3/m$	$P6_3/m$	

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
177	D_6^1	$(c:(a/a))\cdot 2:6$	$C62$	$C622$	$P622$	$P622$	
178	D_6^2	$(c:(a/a))\cdot 2:6_1$	$C6_12$	$C6_122$	$P6_122$	$P6_122$	
179	D_6^3	$(c:(a/a))\cdot 2:6_5$	$C6_52$	$C6_522$	$P6_522$	$P6_522$	
180	D_6^4	$(c:(a/a))\cdot 2:6_2$	$C6_22$	$C6_222$	$P6_222$	$P6_222$	
181	D_6^5	$(c:(a/a))\cdot 2:6_4$	$C6_42$	$C6_422$	$P6_422$	$P6_422$	
182	D_6^6	$(c:(a/a))\cdot 2:6_3$	$C6_32$	$C6_322$	$P6_322$	$P6_322$	
183	C_{6v}^1	$(c:(a/a)):m\cdot 6$	$C6mm$	$C6mm$	$P6mm$	$P6mm$	
184	C_{6v}^2	$(c:(a/a)):\tilde{c}\cdot 6$	$C6cc$	$C6cc$	$P6cc$	$P6cc$	
185	C_{6v}^3	$(c:(a/a)):\tilde{c}\cdot 6_3$	$C6cm$	$C6_3cm$	$P6_3cm$	$P6_3cm$	
186	C_{6v}^4	$(c:(a/a)):m\cdot 6_3$	$C6mc$	$C6_3mc$	$P6_3mc$	$P6_3mc$	
187	D_{3h}^1	$(c:(a/a)):m\cdot 3:m$	$C\bar{6}m2$	$C\bar{6}m2$	$P\bar{6}m2$	$P\bar{6}m2$	
188	D_{3h}^2	$(c:(a/a)):\tilde{c}\cdot 3:m$	$C\bar{6}c2$	$C\bar{6}c2$	$P\bar{6}c2$	$P\bar{6}c2$	
189	D_{3h}^3	$(c:(a/a))\cdot m:3\cdot m$	$H\bar{6}m2$	$H\bar{6}m2$	$P\bar{6}2m$	$P\bar{6}2m$	
190	D_{3h}^4	$(c:(a/a))\cdot m:3\cdot\tilde{c}$	$H\bar{6}c2$	$H\bar{6}c2$	$P\bar{6}2c$	$P\bar{6}2c$	
191	D_{6h}^1	$(c:(a/a))\cdot m:6\cdot m$	$C6/mmm$	$C6/m\ 2/m\ 2/m$	$P6/mmm$	$P6/m\ 2/m\ 2/m$	
192	D_{6h}^2	$(c:(a/a))\cdot m:6\cdot\tilde{c}$	$C6/mcc$	$C6/m\ 2/c\ 2/c$	$P6/mcc$	$P6/m\ 2/c\ 2/c$	
193	D_{6h}^3	$(c:(a/a))\cdot m:6_3\cdot\tilde{c}$	$C6/mcm$	$C6_3/m\ 2/c\ 2/m$	$P6_3/mcm$	$P6_3/m\ 2/c\ 2/m$	
194	D_{6h}^4	$(c:(a/a))\cdot m:6_3\cdot m$	$C6/mmc$	$C6_3/m\ 2/m\ 2/c$	$P6_3/mmc$	$P6_3/m\ 2/m\ 2/c$	
195	T^1	$(a:(a/a)):2/3$	$P23$	$P23$	$P23$	$P23$	
196	T^2	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):2/3$	$F23$	$F23$	$F23$	$F23$	
197	T^3	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):2/3$	$I23$	$I23$	$I23$	$I23$	
198	T^4	$(a:(a:a)):2_1//3$	$P2_13$	$P2_13$	$P2_13$	$P2_13$	
199	T^5	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):2_1//3$	$I2_13$	$I2_13$	$I2_13$	$I2_13$	
200	T_h^1	$(a:(a:a))\cdot m/\tilde{6}$	$Pm3$	$P2/m\ \bar{3}$	$Pm\bar{3}$	$P2/m\ \bar{3}$	$Pm3$ (*IT*, 1952)
201	T_h^2	$(a:(a:a))\cdot\widetilde{ab}/\tilde{6}$	$Pn3$	$P2/n\ \bar{3}$	$Pn\bar{3}$	$P2/n\ \bar{3}$	$Pn3$ (*IT*, 1952)
202	T_h^3	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right)\cdot m/\tilde{6}$	$Fm3$	$F2/m\ \bar{3}$	$Fm\bar{3}$	$F2/m\ \bar{3}$	$Fm3$ (*IT*, 1952)
203	T_h^4	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right)\cdot\tfrac{1}{2}ab/\tilde{6}$	$Fd3$	$F2/d\ \bar{3}$	$Fd\bar{3}$	$F2/d\ \bar{3}$	$Fd3$ (*IT*, 1952)
204	T_h^5	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right)\cdot m/\tilde{6}$	$Im3$	$I2/m\ \bar{3}$	$Im\bar{3}$	$I2/m\ \bar{3}$	$Im3$ (*IT*, 1952)
205	T_h^6	$(a:(a:a))\cdot\tilde{a}/\tilde{6}$	$Pa3$	$P2_1/a\ \bar{3}$	$Pa\bar{3}$	$P2_1/a\ \bar{3}$	$Pa3$ (*IT*, 1952)
206	T_h^7	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right)\cdot\tilde{a}/\tilde{6}$	$Ia3$	$I2_1/a\ \bar{3}$	$Ia\bar{3}$	$I2_1/a\ \bar{3}$	$Ia3$ (*IT*, 1952)
207	O^1	$(a:(a:a)):4/3$	$P43$	$P432$	$P432$	$P432$	
208	O^2	$(a:(a:a)):4_2//3$	$P4_23$	$P4_232$	$P4_232$	$P4_232$	
209	O^3	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4/3$	$F43$	$F432$	$F432$	$F432$	
210	O^4	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4_1//3$	$F4_13$	$F4_132$	$F4_132$	$F4_132$	
211	O^5	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4/3$	$I43$	$I432$	$I432$	$I432$	
212	O^6	$(a:(a:a)):4_3//3$	$P4_33$	$P4_332$	$P4_332$	$P4_332$	
213	O^7	$(a:(a:a)):4_1//3$	$P4_13$	$P4_132$	$P4_132$	$P4_132$	
214	O^8	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4_1//3$	$I4_13$	$I4_132$	$I4_132$	$I4_132$	

Table 3.3.3.1 (continued)

No.	Schoen-flies symbol	Shubnikov symbol	Symbols of *International Tables* 1935 Edition Short	1935 Edition Full	Present Edition Short	Present Edition Full	Comments†
215	T_d^1	$(a:(a:a)):\tilde{4}/3$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	
216	T_d^2	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):\tilde{4}/3$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	
217	T_d^3	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):\tilde{4}/3$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	
218	T_d^4	$(a:(a:a)):\tilde{4}//3$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	
219	T_d^5	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):\tilde{4}//3$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	
220	T_d^6	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):\tilde{4}//3$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	
221	O_h^1	$(a:(a:a)):4/\tilde{6}\cdot m$	$Pm3m$	$P4/m\ \bar{3}\ 2/m$	$Pm\bar{3}m$	$P4/m\ \bar{3}\ 2/m$	$Pm3m$ (*IT*, 1952)
222	O_h^2	$(a:(a:a)):4/\tilde{6}\cdot\widetilde{abc}$	$Pn3n$	$P4/n\ \bar{3}\ 2/n$	$Pn\bar{3}n$	$P4/n\ \bar{3}\ 2/n$	$Pn3n$ (*IT*, 1952)
223	O_h^3	$(a:(a:a)):4_2//\tilde{6}\cdot\widetilde{abc}$	$Pm3n$	$P4_2/m\ \bar{3}\ 2/n$	$Pm\bar{3}n$	$P4_2/m\ \bar{3}\ 2/n$	$Pm3n$ (*IT*, 1952)
224	O_h^4	$(a:(a:a)):4_2//\tilde{6}\cdot m$	$Pn3m$	$P4_2/n\ \bar{3}\ 2/m$	$Pn\bar{3}m$	$P4_2/n\ \bar{3}\ 2/m$	$Pn3m$ (*IT* ,1952)
225	O_h^5	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot m$	$Fm3m$	$F4/m\ \bar{3}\ 2/m$	$Fm\bar{3}m$	$F4/m\ \bar{3}\ 2/m$	$Fm3m$ (*IT*, 1952)
226	O_h^6	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot\tilde{c}$	$Fm3c$	$F4/m\ \bar{3}\ 2/c$	$Fm\bar{3}c$	$F4/m\ \bar{3}\ 2/c$	$Fm3c$ (*IT*, 1952)
227	O_h^7	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a(a:a)\right):4_1//\tilde{6}\cdot m$	$Fd3m$	$F4_1/d\ \bar{3}\ 2/m$	$Fd\bar{3}m$	$F4_1/d\ \bar{3}\ 2/m$	$Fd3m$ (*IT*, 1952)
228	O_h^8	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:a:(a:a)\right):4_1//\tilde{6}\cdot\tilde{c}$	$Fd3c$	$F4_1/d\ \bar{3}\ 2/c$	$Fd\bar{3}c$	$F4_1/d\ \bar{3}\ 2/c$	$Fd3c$ (*IT*, 1952)
229	O_h^9	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4/\tilde{6}\cdot m$	$Im3m$	$I4/m\ \bar{3}\ 2/m$	$Im\bar{3}m$	$I4/m\ \bar{3}\ 2/m$	$Im3m$ (*IT*, 1952)
230	O_h^{10}	$\left(\frac{a+b+c}{2}\Big/a:(a:a)\right):4_1//\tilde{6}\cdot\frac{1}{2}\widetilde{abc}$	$Ia3d$	$I4_1/a\ \bar{3}\ 2/d$	$Ia\bar{3}d$	$I4_1/a\ \bar{3}\ 2/d$	$Ia3d$ (*IT*, 1952)

† Abbreviations used in the column *Comments*: *IT*, 1952: *International Tables for X-ray Crystallography,* Vol. I (1952); Sh–K; Shubnikov & Koptsik (1972). Note that this table contains only one notation for the *b*-unique setting and one notation for the *c*-unique setting in the monoclinic case, always referring to cell choice 1 of the space-group tables.

3.3.3.5. Systematic absences

Hermann (1928*a*) emphasized that the short symbols permit the derivation of systematic absences of X-ray reflections caused by the glide/screw parts of the symmetry operations. If $\boldsymbol{h} = (hkl)$ describes the X-ray reflection and $(\boldsymbol{W}, \boldsymbol{w})$ is the matrix representation of a symmetry operation, the matrix can be expanded as follows:

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w}_g + \mathbf{w}_l) = (\boldsymbol{W}, \begin{pmatrix} w_{g,1} \\ w_{g,2} \\ w_{g,3} \end{pmatrix} + \boldsymbol{w}_l).$$

The absence of a reflection is governed by the relation (i) $\boldsymbol{h}\cdot\boldsymbol{W} = \boldsymbol{h}$ and the scalar product (ii) $\boldsymbol{h}\cdot\boldsymbol{w}_g = hw_{g,1} + kw_{g,2} + lw_{g,3}$. A reflection $\boldsymbol{h}$ is absent if condition (i) holds and the scalar product (ii) is not an integer. The calculation must be made for all generators and indicators of the short symbol. Systematic absences, introduced by the further symmetry operations generated, are obtained by the combination of the extinction rules derived for the generators and indicators.

Example: Space group $D_4^{10} = I4_122$ (98)

The generators of the space group are the integral translations and the centring translation $x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$, the rotation 2 in direction [100]: $x, \bar{y}, \bar{z}$ and the rotation 2 in direction [$1\bar{1}0$]: $\bar{y}, \bar{x}, \bar{z}-\frac{1}{4}$. The combination of the two generators gives the operation corresponding to the indicator, namely $\bar{y}, x, z+\frac{1}{4}$, which represents a fourfold screw rotation in the direction [001].

The integral translations imply no restriction because the scalar product is always an integer. For the centring, condition (i) with $\boldsymbol{W} = \boldsymbol{I}$ holds for all reflections (integral condition), but the scalar product (ii) is an integer only for $h+k+l = 2n$. Thus, reflections hkl with $h+k+l \neq 2n$ are absent. The screw rotation 4 has the screw part $\boldsymbol{w}_g = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$. Only 00$l$ reflections obey condition (i) (serial extinction). An integral value for the scalar product (ii) requires $l = 4n$. The twofold axes in the directions [100] and [1$\bar{1}$0] do not imply further absences because $\boldsymbol{w}_g = \boldsymbol{o}$.

Detailed discussion of the theoretical background of conditions for possible general reflections and their derivation is given in Chapter 1.6.

3.3.3.6. Generalized symmetry

The international symbols can be suitably modified to describe generalized symmetry, *e.g.* colour groups, which occur when the symmetry operations are combined with changes of physical properties. For the description of antisymmetry (or 'black–white' symmetry), the symbols of the Bravais lattices are supplemented by additional letters for centrings accompanied by a change in colour. For symmetry operations that are not translations, a prime is added to the usual symbol if a change of colour takes place. A complete description of the symbols and a detailed list of references are given by Koptsik (1966). The Shubnikov symbols have not been extended to colour symmetry.

An introduction to the structure, properties and symbols of magnetic subperiodic and magnetic space groups is given in Chapter 3.6.

3.3.4. Changes introduced in space-group symbols since 1935

Before the appearance of the first edition of *International Tables* in 1935, different notations for space groups were in use. A summary and comparative tables may be found in the introduction to that edition. The international notation was proposed by Hermann (1928*a*,*b*) and Mauguin (1931), who used the concept of lattice symmetry directions (see Section 3.3.1) and gave preference to reflections or glide reflections as generators. Considerable changes to the original Hermann–Mauguin short symbols were made in *IT* (1952).

The most important change refers to the symmetry directions. In the original Hermann–Mauguin symbols [*IT* (1935)], the distribution of symmetry elements is prescribed by the point-group symbol in the traditional setting, for example $\bar{4}2m$ (not $\bar{4}m2$) but $\bar{6}m2$ (not $\bar{6}2m$). This procedure sometimes implies the use of a larger unit cell than would be necessary. In *IT* (1952) and in the present series, however, the lattice symmetry directions always refer to the conventional cell (*cf.* Chapter 3.1) of the Bravais lattice. The results of this change are (*a*) different symbols for centring types and (*b*) different sequences of the symbols referring to the point group. These differences occur only in some space groups that have a tetragonal or hexagonal lattice.

Thus, the two different space groups D^1_{2d} and D^5_{2d} were symbolized by $P\bar{4}2m$ and $C\bar{4}2m$ in *IT* (1935) because in both cases the twofold axis had to be connected with the secondary set of symmetry directions. The new international symbols are $P\bar{4}2m$ and $P\bar{4}m2$; since in the point group $4/m\ 2/m\ 2/m$ of the Bravais lattice the secondary and tertiary set cannot be distinguished, the twofold axis in the subgroups $\bar{4}2m$ and $\bar{4}m2$ may occur in either the secondary or the tertiary set. Accordingly, the *C*-centred cell of $D^5_{2d} - C\bar{4}2m$, used in *IT* (1935), was transformed to a primitive one with the twofold axis along the tertiary set, resulting in the symbol $P\bar{4}m2$.

The same considerations hold for $\bar{6}m2$ and $\bar{6}2m$ and for space groups with a hexagonal lattice belonging to the point groups 32, $3m$ and $\bar{3}m$, which can be oriented in two ways with respect to the lattice.

For example, the point group $3m$ has two sets of symmetry directions. If the basis vector **a** is normal to the mirror plane *m*, two hexagonal cells with different centrings are possible:

(i) the hexagonal primitive cell, always described by *C* in *IT* (1935), leads to $C3m = C^1_{3v}$;

(ii) the hexagonal *H*-centred cell, with centring points in $\frac{2}{3}, \frac{1}{3}, 0$ and $\frac{1}{3}, \frac{2}{3}, 0$, leads to $H3m = C^2_{3v}$ (*cf.* Chapter 3.1).

The latter can be transformed to a primitive cell in which the mirror plane is normal to the representative of the tertiary set of the hexagonal lattice. In *IT* (1952) and the present editions, the primitive hexagonal cell is described by *P*. Thus, the above space groups receive the symbols $P3m1 = C^1_{3v}$ and $P31m = C^2_{3v}$.

Further changes are:

(i) In *IT* (1952), symbols for space groups related to the point groups 422, 622 and 432 contain the twofold axis of the tertiary set. The advantage is that these groups can be generated by operations of the secondary and tertiary set. The symbol of the indicator is provided with the appropriate index to identify the screw part, thus fixing the intersection parameter.

(ii) Some standard settings are changed in the monoclinic system. In *IT* (1935), only one setting (*b* unique, one cell choice) was tabulated for the monoclinic space groups. In *IT* (1952), two choices were offered, *b* and *c* unique, each with one cell choice. In the present edition, the two choices (*b* and *c* unique) are retained but for each one three different cells are available. The standard short symbol, however, is that of *IT* (1935) (*b*-unique setting).

(iii) In the short symbols of centrosymmetric space groups in the cubic system, $\bar{3}$ is written instead of 3, *e.g.* $Pm\bar{3}$ instead of $Pm3$ [as in *IT* (1935) and *IT* (1952)].

(iv) Beginning with the fourth edition of this volume (1995), the following five orthorhombic space-group symbols have been modified by introducing the new glide-plane symbol *e*, according to a Nomenclature Report of the IUCr (de Wolff *et al.*, 1992).

Space group No.	39	41	64	67	68
Former symbol:	*Abm*2	*Aba*2	*Cmca*	*Cmma*	*Ccca*
New symbol:	*Aem*2	*Aea*2	*Cmce*	*Cmme*	*Ccce*

The new symbol is indicated in the headline of these space groups. Further details are given in Section 2.1.2.

Difficulties arising from these changes are avoided by selecting the lexicographically first one of the two possible glide parts for the generating operation.

Example: $Aea2 \sim Aba2 = C^{17}_{2v}$ (41)

The generators are

A centring:	$x, y+\frac{1}{2}, z+\frac{1}{2}$	$(1) + (0, \frac{1}{2}, \frac{1}{2})$
glide reflection b_{100}:	$\bar{x}, y+\frac{1}{2}, z$	(4)
or glide reflection c_{100}:	$\bar{x}, y, z+\frac{1}{2}$	$(4) + (0, \frac{1}{2}, \frac{1}{2})$
The first possibility is selected.		
glide reflection a_{010}:	$x+\frac{1}{2}, \bar{y}, z$	(3).

A shift of origin by $(-\frac{1}{4}, -\frac{1}{2}, 0)$ is necessary.

The 1935 symbols and all the changes adopted in the present edition of *International Tables* can be seen in Table 3.3.3.1. Differences in the symbols between *IT* (1952) and the present edition may be found in the last column of this table; *cf.* also Section 2.1.3.4.

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