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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 $\overline{1}$, $\overline{2} \equiv m$, $\overline{3}$ and $\overline{4}$, 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 $\overline{6}$ 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$\overline{1}$]}, representative is [001]; the secondary set of lattice symmetry directions consists of [100], [010], [$\overline{1}\overline{1}$0] and their counter-directions, representative is [100]; the tertiary set of lattice symmetry directions consists of [1$\overline{1}$0], [120], [$\overline{2}\overline{1}$0] and their counter-directions, representative is [1$\overline{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	$\overline{1}$ m $\overline{3}$ $\overline{4}$ $\overline{6}$
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 $4mm$ 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 $3m$ of 432 or $\bar{4}3m$ will be generated.

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

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 $\mathbf{w}$ 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.

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 $\odot$, $\bigcirc\!\!\!\!\!:\;$, //. 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 unifi-