International Tables for Crystallography (2016). Vol. A, Section 3.3.2.4, pp. 779–780.

(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.

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 **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 $0\le m<k$ 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 $\odot$, $\bigcirc\kern-0.72em:\;$, //. 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