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cation, 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 $\bar{6}$.