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$(\boldsymbol{W}, \boldsymbol{w})$ 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)

references