

3.3. SPACE-GROUP SYMBOLS AND THEIR USE

(\mathbf{W} , \mathbf{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 \mathbf{W} on x, y, z , while the second corresponds to the translation part \mathbf{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 $Pccm(000)$.

(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 $Ibam(-\frac{1}{4} - \frac{1}{4} 0)$.

(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 $\mathbf{w}_l = \begin{pmatrix} 0 \\ 0 \\ -\frac{1}{4} \end{pmatrix}$. The expanded symbol $P4_12_12(\frac{1}{4} - \frac{1}{4} - \frac{3}{8})$ 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 $\mathbf{w}_l = \begin{pmatrix} -\frac{1}{2} \\ 0 \\ 0 \end{pmatrix} \equiv \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}$.

No origin shift is necessary. The expanded symbol is $P2_13(000)$.

(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 $\mathbf{w}_l = \begin{pmatrix} -\frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix}$. No origin shift is necessary. The expanded symbol is $P4_132(000)$.

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

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

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 $\bar{6}$.