12.3. Properties of the international symbols

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12.3.1. 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 $\boldsymbol{w}_l = (0, 0, -m/n)$; 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 $\boldsymbol{w}_l = (-m/n, 0, 0)$ 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 $w_l = (-m/n, m/n, m/n)$ 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 '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 a matrix $\boldsymbol{q} = \langle q^1, q^2, q^3\rangle$ to the short space-group symbol. The shift of origin can be performed easily, for only the translation parts have to be changed. The new matrix of the translation part can be obtained by

$$\boldsymbol{w}' = \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I}) \cdot \boldsymbol{q}.$$

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 a pair of row matrices. The first one consists of the coordinates of a point in general position after the application of $\boldsymbol{W}$ on $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$; the second represents the translation part $\begin{pmatrix} w^1 \\ w^2 \\ w^3 \end{pmatrix}$. In the following, both are written as a row. The sum of both matrices is tabulated as *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 11.2.2.1 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 2.2.9 and 2.2.11. 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):

$$\begin{array}{lll} \text{glide reflection} & c_{[100]} : & (\bar{x}yz, 00\tfrac{1}{2}) \quad (8) \\ \text{glide reflection} & c_{[010]} : & (x\bar{y}z, 00\tfrac{1}{2}) \quad (7) \\ \text{reflection} & m_{[001]} : & (xy\bar{z}, 000) \quad (6). \end{array}$$

No shift of origin is necessary. The extended 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:

$$\begin{array}{lll} I \text{ centring} & : (xyz, \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) & (1) + (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) \\ \text{glide reflection } b_{[100]} & : (\bar{x}yz, 0\tfrac{1}{2}0) & (8) \\ \text{glide reflection } a_{[010]} & : (x\bar{y}z, \tfrac{1}{2}00) & (7) \\ \text{reflection} \quad m_{[001]} & : (xy\bar{z}, 000) & (6). \end{array}$$

To obtain the tabulated general position, a shift of origin by $(-\frac{1}{4}, -\frac{1}{4}, 0)$ is necessary, the extended 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:

$$\begin{array}{lll} \text{screw rotation } 2_1 \text{ in } [100] & : (x\bar{y}\bar{z}, \tfrac{1}{2}00) & (6) \\ \text{rotation} \quad 2 \text{ in } [1\bar{1}0] & : (\bar{y}\bar{x}\bar{z}, 00\tfrac{1}{4}) & (8). \end{array}$$

According to rule (iii), the location part of the first generator, referring to the secondary set of symmetry direction, is equal to zero. For the second generator, the screw part is equal to zero. The location part is $(0, 0, -\frac{1}{4})$.

The extended 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

$$\begin{array}{lll} \text{rotation 3 in } [111] & : (zxy, 000) & (5) \\ \text{screw rotation } 2_1 \text{ in } [001] & : (\bar{x}\bar{y}z, \tfrac{1}{2}0\tfrac{1}{2}) & (2). \end{array}$$

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 $(0, 0, \frac{1}{2})$, the location part $\boldsymbol{w}_l$ is $(-\frac{1}{2}, 0, 0) \equiv (\frac{1}{2}, 0, 0)$. No origin shift is necessary. The extended symbol is $P2_13\langle 000\rangle$.

(5) $P4_132 = O^7$ (213)

Besides the integral translations, the generators given by the symbol are:

$$\begin{array}{lll} \text{rotation 3 in } [111] & : (zxy, 000) & (5) \\ \text{rotation 2 in } [110] & : (yx\bar{z}, -\tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{4}) & (13). \end{array}$$

The screw part of the twofold axis is zero. According to rule (iv), the location part $\boldsymbol{w}_l$ is $(-\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. No origin shift is necessary. The extended symbol is $P4_132\langle 000\rangle$.

12.3.2. 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

references