

## 3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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

$$\left( \frac{a+b+c}{2} / c : (a:b) \right),$$

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  $\mathbf{c}$ , which is orthogonal to the perpendicular pair  $\mathbf{a}$  and  $\mathbf{b}$ . 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  $(\mathbf{a}, \mathbf{b})$  plane, there is a glide plane  $\bar{a}b$  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  $\mathbf{c}$ , the latter is chosen as generator. The third generator can be a glide plane  $c$  perpendicular to  $\mathbf{b}$ . Thus the Shubnikov symbol of  $D_{2h}^{26}$  is

$$\left( \frac{a+b+c}{2} / c : (a:b) \right) \cdot m : 2 \cdot \bar{c}.$$

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  $\mathbf{W}$  of the generating operations  $(\mathbf{W}, \mathbf{w})$ .

The modified symbols of the generators determine the glide/screw parts  $\mathbf{w}_g$  of  $\mathbf{w}$ . To find the location parts  $\mathbf{w}_l$  of  $\mathbf{w}$ , 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  $\mathbf{w}_l = \begin{pmatrix} 0 \\ 0 \\ -m/n \end{pmatrix}$ ; 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

$\mathbf{w}_l = \begin{pmatrix} -m/n \\ 0 \\ 0 \end{pmatrix}$  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

$\mathbf{w}_l = \begin{pmatrix} -m/n \\ m/n \\ m/n \end{pmatrix}$  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)]

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

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