(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)