$Pmma \sim Pmmb$, $Pnma \sim Pmnb$, $Pmna \sim Pnmb$ and $Pnna \sim Pnnb$.

12.3.4. 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.* Chapter 12.4), 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 12.3.4.1 in which the short symbols are listed for all space groups. A table for all settings may be found in Chapter 4.3.

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 *mm*2, 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 Chapter 4.1].

12.3.5. Systematic absences

Hermann (1928) emphasized that the short symbols permit the derivation of systematic absences of X-ray reflections caused by the glide/screw parts of the symmetry operations. If $\boldsymbol{H} = (h, k, l)$ describes the X-ray reflection and $(\boldsymbol{W}, \boldsymbol{w})$ is the matrix representation of a symmetry operation, the matrix can be expanded as follows:

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w}_g + \mathbf{w}_l) = (\boldsymbol{W}, \begin{pmatrix} w_g^1 \\ w_g^2 \\ w_g^3 \end{pmatrix} + \boldsymbol{w}_l).$$

The absence of a reflection is governed by the relation (i) $\boldsymbol{H} \cdot \boldsymbol{W} = \boldsymbol{H}$ and the scalar product (ii) $\boldsymbol{H} \cdot \boldsymbol{w}_g = hw_g^1 + kw_g^2 + lw_g^3$. A reflection $\boldsymbol{H}$ is absent if condition (i) holds and the scalar product (ii) is not an integer. The calculation must be made for all generators and indicators of the short symbol. Systematic absences, introduced by the further symmetry operations generated, are obtained by the combination of the extinction rules derived for the generators and indicators.

Example: Space group $D_4^{10} = I4_122$ (98)

The generators of the space group are the integral translations and the centring translation $(xyz, \frac{1}{2}\frac{1}{2}\frac{1}{2})$, the rotation 2 in direction [100]: $(x\bar{y}\bar{z}, 000)$ and the rotation 2 in direction $[1\bar{1}0]$: $(\bar{y}\bar{x}\bar{z}, 00-\frac{1}{4})$. The operation corresponding to the indicator is the product of the two generators:

$$(x\bar{y}\bar{z}, 000)\ (\bar{y}\bar{x}\bar{z}, 00-\tfrac{1}{4}) = (\bar{y}xz, 00\tfrac{1}{4}).$$

The integral translations imply no restriction because the scalar product is always an integer. For the centring, condition (i) with $\boldsymbol{W} = \boldsymbol{I}$ holds for all reflections (integral condition), but the scalar product (ii) is an integer only for $h + k + l = 2n$. Thus, reflections *hkl* with $h + k + l \neq 2n$ are absent. The screw rotation 4 has the screw part $\boldsymbol{w}_g = (0, 0, \frac{1}{4})$. Only 00*l* reflections obey condition (i) (serial extinction). An integral value for the scalar product (ii) requires $l = 4n$. The twofold axes in the directions [100] and $[1\bar{1}0]$ do not imply further absences because $\boldsymbol{w}_g = \mathbf{0}$.

12.3.6. Generalized symmetry

The international symbols can be suitably modified to describe generalized symmetry, *e.g.* colour groups, which occur when the symmetry operations are combined with changes of physical properties. For the description of antisymmetry (or 'black–white' symmetry), the symbols of the Bravais lattices are supplemented by additional letters for centrings accompanied by a change in colour. For symmetry operations that are not translations, a prime is added to the usual symbol if a change of colour takes place. A complete description of the symbols and a detailed list of references are given by Koptsik (1966). The Shubnikov symbols have not been extended to colour symmetry.

references