3.3. SPACE-GROUP SYMBOLS AND THEIR USE

(i) components that represent the type of the generating operation, which are called *generators*;

(ii) components that are not used as generators but that serve to fix the directions of other symmetry elements (Hermann, 1931), and which are called *indicators*.

The generating matrices are uniquely defined by (i) and (ii) if it is assumed that they describe motions with counterclockwise rotational sense about the representative direction looked at end on by the observer. The symbols 2, 4, $\bar{4}$, 6 and $\bar{6}$ referring to direction [001] are indicators when the point-group symbol uses three sets of lattice symmetry directions. For instance, in 4*mm* the indicator 4 fixes the directions of the mirrors normal to [100] and [1$\bar{1}$0].

Note: The generation of (*a*) point group 432 by a rotation 3 around [111] and a rotation 2 and (*b*) point group $\bar{4}$3*m* by 3 around [111] and a reflection *m* is only possible if the representative direction of the tertiary set is changed from [1$\bar{1}$0] to [110]; otherwise only the subgroup 32 or 3*m* of 432 or $\bar{4}$3*m* will be generated.

3.3.2. Space-group symbols

3.3.2.1. Introduction

Each space group is related to a crystallographic point group. Space-group symbols, therefore, can be obtained by a modification of point-group symbols. The simplest modification which merely gives an enumeration of the space-group types (*cf.* Section 1.3.4.1) has been used by Schoenflies. The Shubnikov and Hermann–Mauguin symbols, however, reveal the glide or screw components of the symmetry operations and are designed in such a way that the nature of the symmetry elements and their relative locations can be deduced from the symbol. [A detailed discussion and listings of computer-adapted space-group symbols implemented in crystallographic software, such as the so-called *Hall symbols* (Hall, 1981*a,b*) or *explicit symbols* (Shmueli, 1984), can be found in Chapter 1.4 of *International Tables for Crystallography*, Volume B (2008).]

3.3.2.2. Schoenflies symbols

Space groups related to one point group are distinguished by adding a numerical superscript to the point-group symbol. Thus, the space groups related to the point group C_2 are called C_2^1, C_2^2, C_2^3.

3.3.2.3. The role of translation parts in the Shubnikov and Hermann–Mauguin symbols

A crystallographic symmetry operation W (*cf.* Chapter 1.2) is described by a pair of matrices

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{w})(\boldsymbol{W}, \boldsymbol{o}).$$

W is called the *rotation part*, **w** describes the *translation part* and determines the translation vector **w** of the operation. The translation part **w** can be decomposed into a *glide/screw part* $\boldsymbol{w}_g$ and a *location part* $\boldsymbol{w}_l$: $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$; here, $\boldsymbol{w}_l$ determines the location of the corresponding symmetry element with respect to the origin. The glide/screw part $\boldsymbol{w}_g$ may be derived by projecting **w** on the space invariant under W, *i.e.* for rotations and reflections **w** is projected on the corresponding rotation axis or mirror plane. With matrix notation, $\boldsymbol{w}_g$ is determined by $(\boldsymbol{W}, \boldsymbol{w})^k = (\boldsymbol{I}, \boldsymbol{t})$ and $\boldsymbol{w}_g = (m/k)\boldsymbol{t}_1$, where k is the order of W, the integers m are restricted by $0 \le m < k$ and $\boldsymbol{t}_1$ is the shortest lattice vector in the

Table 3.3.2.1

Symbols of glide planes in the Shubnikov and Hermann–Mauguin space-group symbols

Glide plane perpendicular to	Glide vector	Shubnikov symbol	Hermann–Mauguin symbol
b or **c**	$\frac{1}{2}\mathbf{a}$	$\tilde{a}$	*a*
a or **c**	$\frac{1}{2}\mathbf{b}$	$\tilde{b}$	*b*
a or **b** or **a** − **b**	$\frac{1}{2}\mathbf{c}$	$\tilde{c}$	*c*
c	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\widetilde{ab}$	*n*
a	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$	$\widetilde{bc}$	*n*
b	$\frac{1}{2}(\mathbf{c}+\mathbf{a})$	$\widetilde{ac}$	*n*
a − **b**	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\widetilde{abc}$	*n*
c	$\frac{1}{4}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}\widetilde{ab}$	*d*
a	$\frac{1}{4}(\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{bc}$	*d*
b	$\frac{1}{4}(\mathbf{c}+\mathbf{a})$	$\frac{1}{2}\widetilde{ac}$	*d*
a − **b**	$\frac{1}{4}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{abc}$	*d*
a + **b**	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$		*d*

direction of **t** (for details, *cf.* Sections 1.2.2.4 and 1.5.4.1). Space groups contain sets of screw and rotation axes or glide and mirror planes. A screw rotation is symbolized by k_m. The Shubnikov notation and the international notation use the same symbols for screw rotations. The symbols for glide reflections in both notations are listed in Table 3.3.2.1.

If the point-group symbol contains only one generator, the related space group is described completely by the Bravais lattice and a symbol corresponding to that of the point group in which rotations and reflections are replaced by screw rotations or glide reflections, if necessary. If, however, two or more operations generate the point group, it is necessary to have information on the mutual orientations and locations of the corresponding space-group symmetry elements, *i.e.* information on the location components $\boldsymbol{w}_l$. This is described in the following sections.

3.3.2.4. Shubnikov symbols

For the description of the mutual orientation of symmetry elements, the same symbols as for point groups are applied. In space groups, however, the symmetry elements need not intersect. In this case, the orientational symbols · (dot), : (colon), / (slash) are modified to ⊙, ⊙, //. The space-group symbol starts with a description of the lattice defined by the basis **a**, **b**, **c**. For centred cells, the vectors to the centring points are given first. The same letters are used for basis vectors related by symmetry. The relative orientations of the vectors are denoted by the orientational symbols introduced above. The description of the lattice given in parentheses is followed by symbols of the generating elements of the related point group. If necessary, the symbols of the symmetry operations are modified to indicate their glide/screw parts. The first generator is separated from the lattice description by an orientation symbol. If this generator represents a mirror or glide plane, the dot connects the plane with the last two vectors whereas the colon refers only to the last vector. If the generator represents a rotation or a rotoreflection, the colon orients the related axis perpendicular to the plane given by the last two vectors whereas the dot refers only to the last vector. Two generators are separated by the symbols mentioned above to denote their relative orientations and sites. To make this description unique for space groups related to point group $O_h \equiv 6/4$ with Bravais lattices *cP* and *cF*, it is necessary to use three generators instead of two: $4/\tilde{6} \cdot m$. For the sake of unifi-

references