International Tables for Crystallography (2016). Vol. A, Section 1.4.2.4, pp. 55–56.

$x, \frac{3}{4}, z$; $x, \frac{5}{4}, z$; ...; $x, (2u_2 + 1)/4, z$. As usual, the symmetry operation with $u_1 = u_2 = u_3 = 0$, *i.e.* $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2} = \{m_{010}|0, \frac{1}{2}, \frac{1}{2}\}$, is taken as a coset representative of the coset of glide reflections.

The coordinate triplets of the general-position block of $P2_1/c$ (unique axis b, cell choice 1) (*cf.* Fig. 1.4.2.1) correspond to the coset representatives of the decomposition of the group listed in the first line of Table 1.4.2.6.

When the space group is referred to a primitive basis (which is always done for '*P*' space groups), each coordinate triplet of the general-position block corresponds to one coset of $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$, *i.e.* the *multiplicity* of the general position and the number of cosets is the same. If, however, the space group is referred to a centred cell, then the complete set of general-position coordinate triplets is obtained by the combinations of the listed coordinate triplets with the centring translations. In this way, the total number of coordinate triplets per conventional unit cell, *i.e.* the multiplicity of the general position, is given by the product $[i] \times [p]$, where $[i]$ is the index of $\mathcal{T}_{\mathcal{G}}$ in $\mathcal{G}$ and $[p]$ is the index of the group of integer translations in the group $\mathcal{T}_{\mathcal{G}}$ of all (integer and centring) translations.

Example

The listing of the general position for the space–group type *Fmm*2 (42) of the space-group tables is reproduced in Fig. 1.4.2.2. The four entries, numbered (1) to (4), are to be taken as they are printed [indicated by (0, 0, 0)+]. The additional 12 more entries are obtained by adding the centring translations $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$ to the translation parts of the printed entries [indicated by $(0, \frac{1}{2}, \frac{1}{2})+$, $(\frac{1}{2}, 0, \frac{1}{2})+$ and $(\frac{1}{2}, \frac{1}{2}, 0)+$, respectively]. Altogether there are 16 entries, which is announced by the multiplicity of the general position, *i.e.* by the first number in the row. (The additional information specified on the left of the general-position block, namely the Wyckoff letter and the site symmetry, will be dealt with in Section 1.4.4.)

1.4.2.4. Additional symmetry operations and symmetry elements

The symmetry operations of a space group are conveniently partitioned into the cosets with respect to the translation subgroup. All operations which belong to the same coset have the same linear part and, if a single operation from a coset is given, all other operations in this coset are obtained by composition with a translation. However, not all symmetry operations in a coset with respect to the translation subgroup are operations of the same type and, furthermore, they may belong to element sets of different symmetry elements. In general, one can distinguish the following cases:

(i) The composition $W' = tW$ of a symmetry operation W with a translation t is an operation of the same type as W, with the same or a different type of symmetry element.

(ii) The composition $W' = tW$ is an operation of a different type to W with the same or a different type of symmetry element.

In order to distinguish the different cases, a closer analysis of the type of a symmetry operation and its symmetry element is required. These types, however, might be obscured by two obstacles:

(1) The origin in the chosen coordinate system might not lie on the geometric element of the symmetry operation. For example, the symmetry operation represented by the coordinate triplet $\bar{x} + 1, \bar{y} + 1, \bar{z}$ (*cf.* Section 1.4.2.3) is in fact an inversion through the point $1/2, 1/2, 0$ and thus of the same type as the inversion $\{\bar{1}|0\}$ through the origin.

(2) The screw or glide part might not be reduced to a vector within the unit cell. For example, the symmetry operation $\bar{x}, \bar{y}, z + 1$, which is a twofold screw rotation $2\ (0, 0, 1)\ 0, 0, z$ along the c axis, is the composition of the twofold rotation $\bar{x}, \bar{y}, z$ with the lattice translation $t(0, 0, 1)$ along the screw axis. Although the two operations $\bar{x}, \bar{y}, z$ and $\bar{x}, \bar{y}, z + 1$ are of different types, they are coaxial equivalents and belong to the element set of the same symmetry element (*cf.* Section 1.2.3).

These issues can be overcome by decomposing the translation part $\boldsymbol{w}$ of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ into an intrinsic translation part $\boldsymbol{w}_g$ which is fixed by the linear part $\boldsymbol{W}$ of W and thus parallel to the geometric element of W, and a location part $\boldsymbol{w}_l$, which is perpendicular to the intrinsic translation part. Note that the subspace of vectors fixed by $\boldsymbol{W}$ and the subspace perpendicular to this space of fixed vectors are complementary subspaces, *i.e.* their dimensions add up to 3, therefore this decomposition is always possible.

The procedure for determining the intrinsic translation part of a symmetry operation is described in Section 1.2.2.4, and is based on the fact that the kth power of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ with linear part $\boldsymbol{W}$ of order k must be a pure translation, *i.e.* $W^k = (\boldsymbol{I}, \boldsymbol{t})$ for some lattice translation $\boldsymbol{t}$. The *intrinsic translation part* of W is then defined as $\boldsymbol{w}_g = \frac{1}{k}\boldsymbol{t}$.

The difference $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{w}_g$ is perpendicular to $\boldsymbol{w}_g$ and it is called the *location part* of $\boldsymbol{w}$. This terminology is justified by the fact that the location part can be reduced to $\boldsymbol{o}$ by an origin shift, *i.e.* the location part indicates whether the origin of the chosen coordinate system lies on the geometric element of W.

The transformation of point coordinates and matrix–column pairs under an origin shift is explained in detail in Sections 1.5.1.3 and 1.5.2.3, and the complete procedure for determining the additional symmetry operations will be discussed in the context of the synoptic tables in Section 1.5.4. In this section we will restrict ourselves to a detailed discussion of two examples which illustrate typical phenomena.

Example 1

Consider a space group of type *Fmm*2 (42). The information on the general position and on the symmetry operations given in the space-group tables are reproduced in Fig. 1.4.2.2. From this information one deduces that coset representatives with respect to the translation subgroup are the identity element $W_1 = x, y, z$, a rotation $W_2 = \bar{x}, \bar{y}, z$ with the c axis as geometric element, a reflection $W_3 = x, \bar{y}, z$ with the plane $x, 0, z$ as geometric element and a reflection $W_4 = \bar{x}, y, z$ with the plane $0, y, z$ as geometric element (with the indices following the numbering in the table).

Composing these coset representatives with the centring translations $t(0, \frac{1}{2}, \frac{1}{2})$, $t(\frac{1}{2}, 0, \frac{1}{2})$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ gives rise to elements in the same cosets, but with different types of symmetry operations and symmetry elements in several cases.

(i) $(0, \frac{1}{2}, \frac{1}{2})$: The composition of the rotation W_2 with $t(0, \frac{1}{2}, \frac{1}{2})$ results in the symmetry operation $\bar{x}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$, which is a twofold screw rotation with screw axis $0, \frac{1}{4}, z$. This means that both the type of the symmetry operation and the location of the geometric element are changed. Composing the reflection W_3 with $t(0, \frac{1}{2}, \frac{1}{2})$ gives the symmetry operation $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$, which is a c glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the b axis relative to the geometric element of W_3. In the composition of W_4 with $t(0, \frac{1}{2}, \frac{1}{2})$, the translation lies

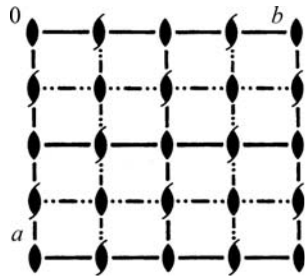

Figure 1.4.2.3
Symmetry-element diagram for space group *Fmm*2 (42) (orthogonal projection along [001]).

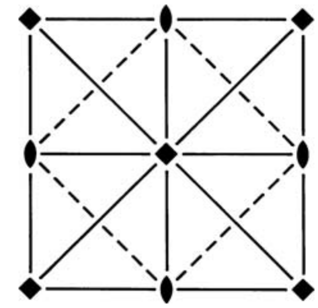

Figure 1.4.2.5
Symmetry-element diagram for space group *P*4*mm* (99) (orthogonal projection along [001]).

in the plane forming the geometric element of W_4. The geometric element of the resulting symmetry operation $\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$ is still the plane $0, y, z$, but the symmetry operation is now an *n* glide, *i.e.* a glide reflection with diagonal glide vector.

(ii) $(\frac{1}{2}, 0, \frac{1}{2})$: Analogous to the first centring translation, the composition of W_2 with $t(\frac{1}{2}, 0, \frac{1}{2})$ results in a twofold screw rotation with screw axis $\frac{1}{4}, 0, z$ as geometric element. The roles of the reflections W_3 and W_4 are interchanged, because the translation vector now lies in the plane forming the geometric element of W_3. Therefore, the composition of W_3 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an *n* glide with the plane $x, 0, z$ as geometric element, whereas the composition of W_4 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is a *c* glide with the plane $\frac{1}{4}, y, z$ as geometric element.

(iii) $(\frac{1}{2}, \frac{1}{2}, 0)$: Because this translation vector lies in the plane perpendicular to the rotation axis of W_2, the composition of W_2 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is still a twofold rotation, *i.e.* a symmetry operation of the same type, but the rotation axis is shifted by $\frac{1}{4}, \frac{1}{4}, 0$ in the *xy* plane to become the axis $\frac{1}{4}, \frac{1}{4}, z$. The composition of W_3 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ results in the symmetry operation $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$, which is an *a* glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the *b* axis relative to the geometric element of W_3. Similarly, the composition of W_4 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is a *b* glide with the plane $\frac{1}{4}, y, z$ as geometric element.

In this example, all additional symmetry operations are listed in the symmetry-operations block of the space-group tables of *Fmm*2 because they are due to compositions of the coset representatives with centring translations.

The additional symmetry operations can easily be recognized in the symmetry-element diagrams (*cf.* Section 1.4.2.5). Fig. 1.4.2.3 shows the symmetry-element diagram of *Fmm*2 for the projection along the *c* axis. One sees that twofold rotation axes alternate with twofold screw axes and that mirror planes alternate with 'double' or *e*-glide planes, *i.e.* glide planes with two glide vectors. For example, the dot–dashed lines at $x = \frac{1}{4}$ and $x = \frac{3}{4}$ in Fig. 1.4.2.3 represent the *b* and *c* glides with normal vector along the *a* axis [for a discussion of *e*-glide notation, see Sections 1.2.3 and 2.1.2, and de Wolff *et al.*, 1992].

Example 2

In a space group of type *P*4*mm* (99), representatives of the space group with respect to the translation subgroup are the powers of a fourfold rotation and reflections with normal vectors along the *a* and the *b* axis and along the diagonals [110] and [1$\bar{1}$0] (*cf.* Fig. 1.4.2.4).

In this case, additional symmetry operations occur although there are no centring translations. Consider for example the reflection W_8 with the plane x, x, z as geometric element. Composing this reflection with the translation $t(1, 0, 0)$ gives rise to the symmetry operation represented by $y+1, x, z$. This operation maps a point with coordinates $x+\frac{1}{2}, x, z$ to $x+1, x+\frac{1}{2}, z$ and is thus a glide reflection with the plane $x+\frac{1}{2}, x, z$ as geometric element and $(\frac{1}{2}, \frac{1}{2}, 0)$ as glide vector. In a similar way, composing the other diagonal reflection with translations yields further glide reflections.

These glide reflections are symmetry operations which are not listed in the symmetry-operations block, although they are clearly of a different type to the operations given there. However, in the symmetry-element diagram as shown in Fig. 1.4.2.5, the corresponding symmetry elements are displayed as diagonal dashed lines which alternate with the solid diagonal lines representing the diagonal reflections.

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*g*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) *m* $x,0,z$	(6) *m* $0,y,z$	(7) *m* $x,\bar{x},z$	(8) *m* x,x,z

Figure 1.4.2.4
General-position and symmetry-operations blocks as given in the space-group tables for space group *P*4*mm* (99).

1.4.2.5. Space-group diagrams

In the space-group tables of Chapter 2.3, for each space group there are at least two diagrams displaying the symmetry (there are more diagrams for space groups of low symmetry). The *symmetry-element* diagram displays the location and orientation of the symmetry elements of the space group. The *general-position* diagrams show the arrangement of a set of symmetry-equivalent points of the general position. Because of the periodicity of the arrangements, the presentation of the contents of one unit cell is sufficient. Both types of diagrams are orthogonal projections of the space-group unit cell onto the plane of projection along a basis vector of the conventional crystallographic coordinate system. The symmetry elements of triclinic, monoclinic and orthorhombic groups are shown in three different projections along the basis vectors.