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equations (1.2.2.1) written for four pairs (point → image point), provided the points X are linearly independent. In fact, because of the special form of the matrix–column pairs, in many cases it is possible to reduce and simplify considerably the calculations necessary for the determination of $(\boldsymbol{W}, \boldsymbol{w})$: the determination of the image points of the origin O and of the three 'coordinate points' A (1, 0, 0), B (0, 1, 0) and C (0, 0, 1) under the symmetry operation is sufficient for the determination of its matrix–column pair.

(1) *The origin*: Let $\tilde{O}$ with coordinates $\tilde{\boldsymbol{o}}$ be the image of the origin O with coordinates $\boldsymbol{o}$, *i.e.* $x_\circ = y_\circ = z_\circ = 0$. Examination of the equations (1.2.2.1) shows that $\tilde{\boldsymbol{o}} = \boldsymbol{w}$, *i.e.* the column $\boldsymbol{w}$ can be determined separately from the coefficients of the matrix $\boldsymbol{W}$.

(2) *The coordinate points*: We consider the point A. Inserting $x = 1, \; y = z = 0$ in equations (1.2.2.1) one obtains $\tilde{x}_i = W_{i1} + w_i$ or $W_{i1} = \tilde{x}_i - w_i$, $i = 1, 2, 3$. The first column of $\boldsymbol{W}$ is separated from the others, and for the solution only the known coefficients w_i have to be subtracted from the coordinates $\tilde{x}_i$ of the image point $\tilde{A}$ of A. Analogously one calculates the coefficients W_{i2} from the image of point B (0, 1, 0) and W_{i3} from the image of point C (0, 0, 1).

Example

What is the pair $(\boldsymbol{W}, \boldsymbol{w})$ for a glide reflection with the plane through the origin, the normal of the glide plane parallel to **c**, and with the glide vector $\boldsymbol{w}_g = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$?

(*a*) *Image of the origin O*: The origin is left invariant by the reflection part of the mapping; it is shifted by the glide part to 1/2, 1/2, 0 which are the coordinates of $\tilde{O}$. Therefore,

$$\boldsymbol{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}.$$

(*b*) *Images of the coordinate points*. Neither of the points A and B are affected by the reflection part, but A is then shifted to 3/2, 1/2, 0 and B to 1/2, 3/2, 0. This results in the equations $3/2 = W_{11} + 1/2$, $1/2 = W_{21} + 1/2$, $0 = W_{31} + 0$ for A and $1/2 = W_{12} + 1/2, 3/2 = W_{22} + 1/2$, $0 = W_{32} + 0$ for B.

One obtains $W_{11} = 1, W_{21} = W_{31} = W_{12} = 0, W_{22} = 1$ and $W_{32} = 0$. Point C: 0, 0, 1 is reflected to 0, 0, −1 and then shifted to 1/2, 1/2, −1.

This means $1/2 = W_{13} + 1/2$, $1/2 = W_{23} + 1/2$, $-1 = W_{33} + 0$ or $W_{13} = W_{23} = 0, W_{33} = -1$.

(*c*) *The matrix–column pair* is thus

$$\boldsymbol{W} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \text{ and } \boldsymbol{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix},$$

which can be represented by the coordinate triplet $x + 1/2, y + 1/2, \bar{z}$ [*cf.* Section 1.2.2.1.1 for the shorthand notation of $(\boldsymbol{W}, \boldsymbol{w})$].

The problem of the determination of $(\boldsymbol{W}, \boldsymbol{w})$ discussed above is simplified if it is reduced to the special case of the derivation of matrix–column pairs of space-group symmetry operations (*General position* block) from their symbols (**Symmetry operations** block) found in the space-group tables of Part 2 of this volume. The main simplification comes from the fact that for all symmetry operations of space groups, the rotation parts $\boldsymbol{W}$ referring to conventional coordinate systems are known and listed in Tables 1.2.2.1 and 1.2.2.2. In this way, given the symbol of the symmetry operation and using the tabulated data, one can write down directly the corresponding rotation part $\boldsymbol{W}$.

The translation part $\boldsymbol{w}$ of the symmetry operation has two components: $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$. The *intrinsic translation part* (or screw or glide component) is given explicitly in the symmetry operation symbol. The *location part* $\boldsymbol{w}_l$ of $\boldsymbol{w}$ is derived from the equations

$$(\boldsymbol{W}, \boldsymbol{w}_l)\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}, \; i.e. \; \boldsymbol{w}_l = (\boldsymbol{I} - \boldsymbol{W})\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}. \quad (1.2.2.20)$$

Here, (x_F, y_F, z_F) are the coordinates of an arbitrary fixed point of the symmetry operation.

Example

Consider the symbol $3^-(1/3, 1/3, -1/3)$ $\bar{x} + 1/3, \bar{x} + 1/6, x$ of the symmetry operation No. (11) of the **Symmetry operations** (0, 0, 0) block of the space group $Ia\bar{3}d$ (230). The corresponding rotational part $\boldsymbol{W}$ is read directly from Table 1.2.2.1:

$$\boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}.$$

The location part $\boldsymbol{w}_l$ is determined by the matrix equations

$$\boldsymbol{w}_l = (\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix})\begin{pmatrix} 1/3 \\ 1/6 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/6 \\ 1/6 \\ 1/3 \end{pmatrix}$$

[*cf.* Equation (1.2.2.20)]. The point with coordinates $x_F = 1/3$, $y_F = 1/6$, $z_F = 0$ is on the screw axis of 3^- $\bar{x} + 1/3, \bar{x} + 1/6, x$, *i.e.* one of the fixed points of the reduced symmetry operation $(\boldsymbol{W}, \boldsymbol{w}_l)$. The translation part $\boldsymbol{w}$ of the matrix–column pair of the symmetry operation is given by

$$\boldsymbol{w} = \boldsymbol{w}_l + \boldsymbol{w}_g = \begin{pmatrix} 1/6 \\ 1/6 \\ 1/3 \end{pmatrix} + \begin{pmatrix} 1/3 \\ 1/3 \\ -1/3 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}.$$

The coordinate triplet $y + 1/2, \bar{z} + 1/2, \bar{x}$, corresponding to the derived matrix–column pair

$$(\boldsymbol{W}, \boldsymbol{w}) = (\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}),$$

coincides exactly with the coordinate triplet listed under No. (11) in the (0, 0, 0) block of the *General positions* of the space group $Ia\bar{3}d$.

1.2.3. Symmetry elements

In the 1970s, when the International Union of Crystallography (IUCr) planned a new series of *International Tables for Crystallography* to replace the series *International Tables for X-ray Crystallography* (1952), there was some confusion about the use of the term *symmetry element*. Crystallographers and mineralogists had used this term for rotation and rotoinversion axes and reflection planes, in particular for the description of the morphology of crystals, for a long time, although there had been no strict definition of 'symmetry element'. With the impact of mathematical group theory in crystallography the term *element* was introduced with another meaning, in which an element is a member of a set, in particular as a group element of a group.

Table 1.2.3.1
Symmetry elements in point and space groups

Name of symmetry element	Geometric element	Defining operation (d.o.)	Operations in element set
Mirror plane	Plane *p*	Reflection through *p*	D.o. and its coplanar equivalents†
Glide plane	Plane *p*	Glide reflection through *p*; 2**v** (not **v**) a lattice-translation vector	D.o. and its coplanar equivalents†
Rotation axis	Line *l*	Rotation around *l*, angle $2\pi/N$, $N = 2, 3, 4$ or 6	1st ... $(N-1)$th powers of d.o. and their coaxial equivalents‡
Screw axis	Line *l*	Screw rotation around *l*, angle $2\pi/N$, $u = j/N$ times shortest lattice translation along *l*, right-hand screw, $N = 2, 3, 4$ or 6, $j = 1, \ldots, (N-1)$	1st ... $(N-1)$th powers of d.o. and their coaxial equivalents‡
Rotoinversion axis	Line *l* and point *P* on *l*	Rotoinversion: rotation around *l*, angle $2\pi/N$, followed by inversion through *P*, $N = 3, 4$ or 6	D.o. and its inverse
Centre	Point *P*	Inversion through *P*	D.o. only

† That is, all glide reflections through the same reflection plane, with glide vectors **v** differing from that of the d.o. (taken to be zero for reflections) by a lattice-translation vector. The glide planes *a*, *b*, *c*, *n*, *d* and *e* are distinguished (*cf.* Table 2.1.2.1). ‡ That is, all rotations and screw rotations around the same axis *l*, with the same angle and sense of rotation and the same screw vector **u** (zero for rotation) up to a lattice-translation vector.

In crystallography these group elements, however, were the symmetry operations of the symmetry groups, not the crystallographic symmetry elements. Therefore, the IUCr Commission on Crystallographic Nomenclature appointed an *Ad-hoc* Committee on the Nomenclature of Symmetry with P. M. de Wolff as Chairman to propose definitions for terms of crystallographic symmetry and for several classifications of crystallographic space groups and point groups.

In the reports of the *Ad-hoc* Committee, de Wolff *et al.* (1989) and (1992) with *Addenda*, Flack *et al.* (2000), the results were published. To define the term *symmetry element* for any symmetry operation was more complicated than had been envisaged previously, in particular for unusual screw and glide components.

According to the proposals of the Committee the following procedure has been adopted (*cf.* also Table 1.2.3.1):

(1) No symmetry element is defined for the identity and the (lattice) translations.

(2) For any symmetry operation of point groups and space groups with the exception of the rotoinversions $\bar{3}$, $\bar{4}$ and $\bar{6}$, the *geometric element* is defined as the *set of fixed points* (the second column of Table 1.2.3.1) of the *reduced operation*, *cf.* equation (1.2.2.17). For reflections and glide reflections this is a plane; for rotations and screw rotations it is a line, for the inversion it is a point. For the rotoinversions $\bar{3}$, $\bar{4}$ and $\bar{6}$ the geometric element is a line with a point (the inversion centre) on this line.

(3) The *element set* (*cf.* the last column of Table 1.2.3.1) is defined as a set of operations that share the same geometric element. The element set can consist of symmetry operations of the same type (such as the powers of a rotation) or of different types, *e.g.* by a reflection and a glide reflection through the same plane. The *defining operation* (d.o.) may be any symmetry operation from the element set that suffices to identify the symmetry element. In most cases, the 'simplest' symmetry operation from the element set is chosen as the d.o. (*cf.* the third column of Table 1.2.3.1). For reflections and glide reflections the element set includes the defining operation and all glide reflections through the same reflection plane but with glide vectors differing by a lattice-translation vector, *i.e.* the so-called *coplanar equivalents*. For rotations and screw rotations of angle $2\pi/k$ the element set is the defining operation, its 1st ... $(k-1)$th powers and all rotations and screw rotations with screw vectors differing from that of the defining operation by a lattice-translation vector, known as *coaxial equivalents*. For a rotoinversion the element set includes the defining operation and its inverse.

(4) The combination of the geometric element and its element set is indicated by the name *symmetry element*. The names of the symmetry elements (first column of Table 1.2.3.1) are combinations of the name of the defining operation attached to the name of the corresponding geometric element. Names of symmetry elements are *mirror plane*, *glide plane*, *rotation axis*, *screw axis*, *rotoinversion axis* and *centre*.[2] This allows such statements as *this point lies on a rotation axis* or *these operations belong to a glide plane*.

Examples

(1) *Glide and mirror planes*. The element set of a glide plane with a glide vector **v** consists of infinitely many different glide reflections with glide vectors that are obtained from **v** by adding any lattice-translation vector parallel to the glide plane, including centring translations of centred cells.

(*a*) It is important to note that if among the infinitely many glide reflections of the element set of the same plane there exists one operation with zero glide vector, then this operation is taken as the *defining operation* (d.o). Consider, for example, the symmetry operation $x+1/2, y+1/2, -z+1/2$ of *Cmcm* (63) [*General position* (1/2, 1/2, 0) block]. This is an *n*-glide reflection through the plane $x, y, 1/4$. However, the corresponding symmetry element is a mirror plane, as among the glide reflections of the element set of the plane $x, y, 1/4$ one finds the reflection $x, y, -z+1/2$ [symmetry operation (6) of the *General position* (0, 0, 0) block].

(*b*) The symmetry operation $x+5/2, y-7/2, -z+3$ is a glide reflection. Its geometric element is the plane $x, y, 3/2$. Its symmetry element is a glide plane in space group *Pmmn* (59) because there is no lattice translation by which the glide vector can be changed to **o**. If, however, the same mapping is a symmetry operation of space group *Cmmm* (65), then its symmetry element is a reflection plane because the glide vector with components $5/2, -7/2, 0$ can be cancelled through a translation $(2+\frac{1}{2})\mathbf{a}+(-4+\frac{1}{2})\mathbf{b}$, which is a lattice translation in a *C* lattice. Evidently, the correct specification of the symmetry element is possible only with respect to a specific translation lattice.

[2] The proposal to introduce the symbols for the symmetry elements *Em*, *Eg*, *En*, En_j, $E\bar{n}$ and $E\bar{1}$ was not taken up in practice. The printed and graphical symbols of symmetry elements used throughout the space-group tables of Part 2 are introduced in Section 2.1.2 and listed in Tables 2.1.2.1 to 2.1.2.7.

(*c*) Similarly, in *Cmme* (67) with an *a*-glide reflection $x + 1/2, y, \bar{z}$, the *b*-glide reflection $x, y + 1/2, \bar{z}$ also occurs. The geometric element is the plane $x, y, 0$ and the symmetry element is an *e*-glide plane.

In fact, all vectors $(u + \frac{1}{2})\mathbf{a} + v\mathbf{b} + \frac{1}{2}k(\mathbf{a} + \mathbf{b})$, u, v, k integers, are glide vectors of glide reflections through the (001) plane of a space group with a *C*-centred lattice. Among them one finds a glide reflection *b* with a glide vector $\frac{1}{2}\mathbf{b}$ related to $\frac{1}{2}\mathbf{a}$ by the centring translation; an *a*-glide reflection and a *b*-glide reflection share the same plane as a geometric element. Their symmetry element is thus an *e*-glide plane.

(*d*) In general, the *e*-glide planes are symmetry elements characterized by the existence of two glide reflections through the same plane with perpendicular glide vectors and with the additional requirement that at least one glide vector is along a crystal axis (de Wolff *et al.*, 1992). The *e*-glide designation of glide planes occurs only when a centred cell represents the choice of basis (*cf.* Table 2.1.2.2). The 'double' *e*-glide planes are indicated by special graphical symbols on the symmetry-element diagrams of the space groups (*cf.* Tables 2.1.2.3 and 2.1.2.4). For example, consider the space group *I*4*cm* (108). The symmetry operations (8) $y, x, z + 1/2$ [*General position* (0, 0, 0) block] and (8) $y + 1/2, x + 1/2, z$ [*General position* (1/2, 1/2, 1/2) block] are glide reflections through the same x, x, z plane, and their glide vectors $\frac{1}{2}\mathbf{c}$ and $\frac{1}{2}(\mathbf{a} + \mathbf{b})$ are related by the centring (1/2, 1/2, 1/2) translation. The corresponding symmetry element is an *e*-glide plane and it is easily recognized on the symmetry-element diagram of *I*4*cm* shown in Chapter 2.3.

(2) *Screw and rotation axes*. The element set of a screw axis is formed by a screw rotation of angle $2\pi/N$ with a screw vector $\mathbf{u}$, its $(N - 1)$ powers and all its co-axial equivalents, *i.e.* screw rotations around the same axis, with the same angle and sense of rotation, with screw vectors obtained by adding a lattice-translation vector parallel to $\mathbf{u}$.

(*a*) Twofold screw axis $\parallel$ [001] in a primitive cell: the element set is formed by all twofold screw rotations around the same axis with screw vectors of the type $(u + \frac{1}{2})\mathbf{c}$, *i.e.* screw components as $\frac{1}{2}\mathbf{c}$, $-\frac{1}{2}\mathbf{c}$, $\frac{3}{2}\mathbf{c}$ *etc.*

(*b*) The symmetry operation $4 - x, -2 - y, z + 5/2$ is a screw rotation of space group $P222_1$ (17). Its geometric element is the line $2, -1, z$ and its symmetry element is a screw axis.

(*c*) The determination of the complete element set of a geometric element is important for the correct designation of the corresponding symmetry element. For example, the symmetry element of a twofold screw rotation with an axis through the origin is a twofold screw axis in the space group $P222_1$ but a fourfold screw axis in $P4_1$ (76).

(3) *Special case*. In point groups $6/m$, $6/mmm$ and space groups $P6/m$ (175), $P6/mmm$ (191) and $P6/mcc$ (192) the geometric elements of the defining operations $\bar{6}$ and $\bar{3}$ are the same. To make the element sets unique, the geometric elements should not be given just by a line and a point on it, but should be labelled by these operations. Then the element sets and thus the symmetry element are unique (Flack *et al.*, 2000).

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