1.2. Crystallographic symmetry

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1.2.1. Crystallographic symmetry operations

Geometric mappings have the property that for each point P of the space, and thus of the object, there is a uniquely determined point $\tilde{P}$, the *image point*. If also for each image point $\tilde{P}$ there is a uniquely determined preimage or original point P, then the mapping is called *reversible*. Non-reversible mappings are called *projections*, *cf.* Section 1.4.5.

A mapping is called a *motion*, a *rigid motion* or an *isometry* if it leaves all distances invariant (and thus all angles, as well as the size and shape of an object). In this volume the term 'isometry' is used.

Isometries are a special kind of affine mappings. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but distances along the same line are preserved.

A mapping is called a *symmetry operation* of an object if (i) it is an isometry, and (ii) it maps the object onto itself. Instead of 'maps the object onto itself' one frequently says 'leaves the object invariant (as a whole)'.

Real crystals are finite objects in physical space, which because of the presence of impurities and structural imperfections such as disorder, dislocations *etc*. are not perfectly symmetric. In order to describe their symmetry properties, real crystals are modelled as blocks of ideal, infinitely extended periodic structures, known as *ideal crystals* or (ideal) crystal structures. Crystal patterns are models of crystal structures in point space. In other words, while the crystal structure is an infinite periodic spatial arrangement of the atoms (ions, molecules) of which the real crystal is composed, the crystal pattern is the related model of the ideal crystal (crystal structure) consisting of a strictly three-dimensional periodic set of points in point space. If the growth of the ideal crystal is undisturbed, then it forms an *ideal macroscopic crystal* and displays its ideal shape with planar faces.

Both the symmetry operations of an ideal crystal and of a crystal pattern are called *crystallographic symmetry operations*. The symmetry operations of the ideal macroscopic crystal form the finite point group of the crystal, those of the crystal pattern form the (infinite) space group of the crystal pattern. Because of its periodicity, a crystal pattern always has translations among its symmetry operations.

The symmetry operations are divided into two main kinds depending whether they preserve or not the so-called *handedness* or *chirality* of chiral objects. *Isometries of the first kind* or *proper isometries* are those that preserve the handedness of chiral objects: *e.g.* if a right (left) glove is mapped by one of these isometries, then the image is also a right (left) glove of equal size and shape. Isometries that change the handedness, *i.e.* the image of a right glove is a left one, of a left glove is a right one, are called *isometries of the second kind* or *improper isometries*. Improper isometries cannot be performed in space physically but can nevertheless be observed as symmetries of objects.

The notion of *fixed points* is essential for the characterization of symmetry operations. A point P is a *fixed point* of a mapping if it is mapped onto itself, *i.e.* the *image point* $\tilde{P}$ is the same as the original point P: $\tilde{P} = P$. The set of all fixed points of an isometry may be the whole space, a plane in the space, a straight line, a point, or the set may be empty (no fixed point).

Crystallographic symmetry operations are also characterized by their *order*: a symmetry operation W is of *order* k if its application k times results in the identity mapping, *i.e* $\mathsf{W}^k = \mathsf{I}$, where I is the identity operation, and $k > 0$ is the smallest number for which this equation is fulfilled.

There are eight different types of isometries that may be crystallographic symmetry operations:

(1) The *identity operation* I maps each point of the space onto itself, *i.e.* the set of fixed points is the whole space. It is the only operation whose order is 1. The identity operation is a symmetry operation of the first kind. It is a symmetry operation of any object and although trivial, it is indispensable for the group properties of the set of symmetry operations of the object (*cf.* Section 1.1.2).

(2) A *translation* t is characterized by its translation vector $\mathbf{t}$. Under translation every point of space is shifted by $\mathbf{t}$, hence a translation has no fixed point. A translation is a symmetry operation of infinite order as there is no number $k \neq 0$ such that $t^k = \mathsf{I}$ with translation vector $\mathbf{o}$. It preserves the handedness of any chiral object.

(3) A *rotation* is an isometry which leaves one line fixed pointwise. This line is called the *rotation axis*. The degree of rotation about this axis is described by its rotation angle ϕ. Because of the periodicity of crystals, the rotation angles of crystallographic rotations are restricted to $\phi = k \times 2\pi/N$, where N = 2, 3, 4 or 6 and k is an integer which is relative prime to N. A rotation of rotation angle $\phi = k \times 2\pi/N$ is of order N and is called an N-fold rotation. A rotation preserves the handedness of any chiral object.

The rotations are also characterized by their *sense of rotation*. The adopted convention for *positive* (*negative*) sense of rotation follows the mathematical convention for *positive* (*negative*) sense of rotation: the sense of rotation is positive (negative) if the rotation is counter-clockwise (clockwise) when viewed down the rotation axis.

(4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is called the *screw axis*. The translation vector is called the *screw vector* or the *intrinsic translation component* $\mathbf{w}_g$ (of the screw rotation), *cf.* Section 1.2.2.4. A screw rotation has no fixed points because of its translation component. However, the screw axis is invariant pointwise under the so-called *reduced symmetry operation* of the screw rotation: it is the rotation obtained from the screw rotation by removing its intrinsic translation component.

The screw rotation is a proper symmetry operation. If $\phi = 2\pi/N$ is the smallest rotation angle of a screw rotation, then the screw rotation is called N-fold. Owing to its translation component, the order of any screw rotation is infinite. Let $\mathbf{u}$ be the shortest lattice vector in the direction of the screw axis, and $n\mathbf{u}/N$, with $n \neq 0$ and integer, be the screw vector of the screw rotation by the angle ϕ. After N screw rotations with rotation angle $\phi = 2\pi/N$ the crystal pattern has its original orientation but is shifted parallel to the screw axis by the lattice vector $n\mathbf{u}$.

(5) An N-fold *rotoinversion* $\overline{N}$ is an N-fold rotation coupled with an inversion through a point on the rotation axis. This point is called the *centre of the rotoinversion*. For $N \neq 2$ it is the only fixed point. The axis of the rotation is invariant as a whole under the rotoinversion and is called its *rotoinversion axis*. The restrictions on the angles ϕ of the rotational parts are the same as for rotations. The order of an *N-fold* rotoinversion is N for even N and $2N$ for odd N. A rotoinversion changes the handedness by its inversion component: it maps any right-hand glove onto a left-hand one and *vice versa*. Special rotoinversions are those for $N = 1$ and $N = 2$ which are dealt with separately.

The rotoinversions $\overline{N}$ can be described equally as rotoreflections S_N. The N-fold rotation is now coupled with a reflection through a plane which is perpendicular to the rotation axis and cuts the axis in its centre. The following equivalences hold: $\bar{1} = S_2$, $\bar{2} = m = S_1$, $\bar{3} = S_6^{-1}$, $\bar{4} = S_4^{-1}$ and $\bar{6} = S_3^{-1}$. In this volume the description by rotoinversions is chosen.

(6) The *inversion* can be considered as a onefold rotoinversion ($\bar{1}$, $N = 1$) or equally as a twofold rotoreflection S_2. The fixed point is called the *inversion centre*. The inversion is a symmetry operation of the second kind, its order is 2.

(7) A twofold rotoinversion ($N = 2$) is equivalent to a *reflection* or a *reflection through a plane* and is simultaneously a onefold rotoreflection ($\bar{2} = m = S_1$). It is an isometry which leaves the plane perpendicular to the twofold rotoinversion axis fixed pointwise. This plane is called the *reflection plane* or *mirror plane*; it intersects the rotation axis in its centre. Its orientation is described by the direction of its normal vector, *i.e.* of the rotation axis. (Note that in the space-group tables of Part 2 the reflection planes are specified by their locations, and not by their normal vectors, *cf.* Section 1.4.2.1.) The order of a reflection is 2. As for any rotoinversion, the reflection changes the handedness of a chiral object.

(8) A *glide reflection* is a reflection through a plane coupled with a translation parallel to this plane. The translation vector is called the *glide vector* (or the *intrinsic translation component* $\boldsymbol{w}_g$ of the glide reflection, *cf.* Section 1.2.2.4). A glide reflection changes the handedness and has no fixed point. The set of fixed points of the related reduced symmetry operation (*i.e.* the reflection that is obtained by removing the glide component from the glide reflection) is called the *glide plane*. The glide vector of a glide reflection is 1/2 of a lattice vector $\mathbf{t}$ (including centring translations of centred-cell lattice descriptions, *cf.* Table 2.1.1.2). Whereas twice the application of a reflection restores the original position of the crystal pattern, applying a glide reflection twice results in a translation of the crystal pattern with the translation vector $\mathbf{t} = 2\boldsymbol{w}_g$. The order of any glide reflection is infinite.

1.2.2. Matrix description of symmetry operations[1]

1.2.2.1. Matrix–column presentation of isometries

In order to describe mappings analytically one introduces a coordinate system $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$, consisting of three linearly independent (*i.e.* not coplanar) basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ (or $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$) and an origin O. Referred to this coordinate system each point P can be described by three coordinates x, y, z (or x_1, x_2, x_3). A mapping can be regarded as an instruction for how to calculate the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$ of the image point $\widetilde{X}$ from the coordinates x, y, z of the original point X.

The instruction for the calculation of the coordinates of $\widetilde{X}$ from the coordinates of X is simple for an affine mapping and thus for an isometry. The equations are

$$\begin{aligned}\tilde{x} &= W_{11}x + W_{12}y + W_{13}z + w_1\\ \tilde{y} &= W_{21}x + W_{22}y + W_{23}z + w_2\\ \tilde{z} &= W_{31}x + W_{32}y + W_{33}z + w_3,\end{aligned} \qquad (1.2.2.1)$$

where the coefficients W_{ik} and w_j are constant. These equations can be written using the matrix formalism:

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13}\\ W_{21} & W_{22} & W_{23}\\ W_{31} & W_{32} & W_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} + \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix}. \qquad (1.2.2.2)$$

This matrix equation is usually abbreviated by

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}, \qquad (1.2.2.3)$$

where

$$\tilde{\boldsymbol{x}} = \begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix},\quad \boldsymbol{x} = \begin{pmatrix}x\\ y\\ z\end{pmatrix},\quad \boldsymbol{w} = \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix} \text{ and}$$

$$\boldsymbol{W} = \begin{pmatrix} W_{11} & W_{12} & W_{13}\\ W_{21} & W_{22} & W_{23}\\ W_{31} & W_{32} & W_{33}\end{pmatrix}.$$

The matrix $\boldsymbol{W}$ is called the *linear part* or *matrix part* and the column $\boldsymbol{w}$ is the *translation part* or *column part* of the mapping. The rotation parts $\boldsymbol{W}$ referring to conventional coordinate systems of all space-group symmetry operations are listed in Tables 1.2.2.1 and 1.2.2.2 as matrices for point-group symmetry operations.

Very often, equation (1.2.2.3) is written in the form

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} \quad\text{or}\quad \tilde{\boldsymbol{x}} = \{\boldsymbol{W} \,|\, \boldsymbol{w}\}\boldsymbol{x}. \qquad (1.2.2.4)$$

The symbols $(\boldsymbol{W}, \boldsymbol{w})$ and $\{\boldsymbol{W} \,|\, \boldsymbol{w}\}$ which describe the mapping referred to the chosen coordinate system are called the *matrix–column pair* and can be considered as *Seitz symbols* (Seitz, 1935) (*cf.* Section 1.4.2.2 for an introduction to and listings of Seitz symbols of crystallographic symmetry operations).

1.2.2.1.1. Shorthand notation of matrix–column pairs

In crystallography in general, and in this volume in particular, an efficient procedure is used to condense the description of symmetry operations by matrix–column pairs considerably. The so-called *shorthand notation* of the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ consists of a coordinate triplet $W_{11}x + W_{12}y + W_{13}z + w_1$, $W_{21}x + W_{22}y + W_{23}z + w_2$, $W_{31}x + W_{32}y + W_{33}z + w_3$. All coefficients '+1' and the terms with coefficients 0 are omitted, while coefficients '−1' are replaced by '−' and are frequently written on top of the variable: $\bar{x}$ instead of $-x$ *etc.* The following examples illustrate the assignments of the coordinate triplets to the matrix–column pairs.

Examples

(1) The coordinate triplet of $y + 1/2, \bar{x} + 1/2, z + 1/4$ stands for the symmetry operation with the rotation part

[1] With Tables 1.2.2.1 and 1.2.2.2 by H. Arnold.

Table 1.2.2.1
Matrices for point-group symmetry operations and orientation of corresponding geometric elements, referred to a cubic, tetragonal, orthorhombic, monoclinic, triclinic or rhombohedral coordinate system

Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 $0, 0, z$ [001]	$\bar{x}, \bar{y}, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 $0, y, 0$ [010]	$\bar{x}, y, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 0, 0$ [100]	$x, \bar{y}, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
3^+ x, x, x [111]	z, x, y	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	3^+ $x, \bar{x}, \bar{x}$ $[1\bar{1}\bar{1}]$	$\bar{z}, \bar{x}, y$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	3^+ $\bar{x}, x, \bar{x}$ $[\bar{1}1\bar{1}]$	$z, \bar{x}, \bar{y}$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$	3^+ $\bar{x}, \bar{x}, x$ $[\bar{1}\bar{1}1]$	$\bar{z}, x, \bar{y}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$
3^- x, x, x [111]	y, z, x	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	3^- $x, \bar{x}, \bar{x}$ $[1\bar{1}\bar{1}]$	$\bar{y}, z, \bar{x}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}$	3^- $\bar{x}, x, \bar{x}$ $[\bar{1}1\bar{1}]$	$\bar{y}, \bar{z}, x$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	3^- $\bar{x}, \bar{x}, x$ $[\bar{1}\bar{1}1]$	$y, \bar{z}, \bar{x}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}$
			2 $x, x, 0$ [110]	$y, x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 0, x$ [101]	$z, \bar{y}, x$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$	2 $0, y, y$ [011]	$\bar{x}, z, y$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
			2 $x, \bar{x}, 0$ $[1\bar{1}0]$	$\bar{y}, \bar{x}, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $\bar{x}, 0, x$ $[\bar{1}01]$	$\bar{z}, \bar{y}, \bar{x}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	2 $0, y, \bar{y}$ $[01\bar{1}]$	$\bar{x}, \bar{z}, \bar{y}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \end{pmatrix}$
			4^+ $0, 0, z$ [001]	$\bar{y}, x, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	4^+ $0, y, 0$ [010]	$z, y, \bar{x}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	4^+ $x, 0, 0$ [100]	$x, \bar{z}, y$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$
			4^- $0, 0, z$ [001]	$y, \bar{x}, z$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	4^- $0, y, 0$ [010]	$\bar{z}, y, x$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	4^- $x, 0, 0$ [100]	$x, z, \bar{y}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$
$\bar{1}$ $0, 0, 0$	$\bar{x}, \bar{y}, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	m $x, y, 0$ [001]	$x, y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	m $x, 0, z$ [010]	$x, \bar{y}, z$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $0, y, z$ [100]	$\bar{x}, y, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\bar{3}^+$ x, x, x [111]	$\bar{z}, \bar{x}, \bar{y}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$	$\bar{3}^+$ $x, \bar{x}, \bar{x}$ $[1\bar{1}\bar{1}]$	$z, x, \bar{y}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$	$\bar{3}^+$ $\bar{x}, x, \bar{x}$ $[\bar{1}1\bar{1}]$	$\bar{z}, x, y$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\bar{3}^+$ $\bar{x}, \bar{x}, x$ $[\bar{1}\bar{1}1]$	$z, \bar{x}, y$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$\bar{3}^-$ x, x, x [111]	$\bar{y}, \bar{z}, \bar{x}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\bar{3}^-$ $x, \bar{x}, \bar{x}$ $[1\bar{1}\bar{1}]$	$y, \bar{z}, x$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	$\bar{3}^-$ $\bar{x}, x, \bar{x}$ $[\bar{1}1\bar{1}]$	$y, z, \bar{x}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\bar{3}^-$ $\bar{x}, \bar{x}, x$ $[\bar{1}\bar{1}1]$	$\bar{y}, z, x$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
			m $x, \bar{x}, z$ [110]	$\bar{y}, \bar{x}, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $\bar{x}, y, x$ [101]	$\bar{z}, y, \bar{x}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	m $x, y, \bar{y}$ [011]	$x, \bar{z}, \bar{y}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \end{pmatrix}$
			m x, x, z $[1\bar{1}0]$	y, x, z	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m x, y, x $[\bar{1}01]$	z, y, x	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	m x, y, y $[01\bar{1}]$	x, z, y	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
			$\bar{4}^+$ $0, 0, z$ [001]	$y, \bar{x}, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{4}^+$ $0, y, 0$ [010]	$\bar{z}, \bar{y}, x$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\bar{4}^+$ $x, 0, 0$ [100]	$\bar{x}, z, \bar{y}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$
			$\bar{4}^-$ $0, 0, z$ [001]	$\bar{y}, x, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{4}^-$ $0, y, 0$ [010]	$z, \bar{y}, \bar{x}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\bar{4}^-$ $x, 0, 0$ [100]	$\bar{x}, \bar{z}, y$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$

Table 1.2.2.2
Matrices for point-group symmetry operations and orientation of corresponding geometric elements, referred to a hexagonal coordinate system

Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3^+ $0, 0, z$ [001]	$\bar{y}, x-y, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3^- $0, 0, z$ [001]	$y-x, \bar{x}, z$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
2 $0, 0, z$ [001]	$\bar{x}, \bar{y}, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	6^+ $0, 0, z$ [001]	$x-y, x, z$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	6^- $0, 0, z$ [001]	$y, y-x, z$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
2 $x, x, 0$ [110]	$y, x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 0, 0$ [100]	$x-y, \bar{y}, \bar{z}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $0, y, 0$ [010]	$\bar{x}, y-x, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
2 $x, \bar{x}, 0$ [1$\bar{1}$0]	$\bar{y}, \bar{x}, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 2x, 0$ [120]	$y-x, y, \bar{z}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $2x, x, 0$ [210]	$x, x-y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
$\bar{1}$ $0, 0, 0$	$\bar{x}, \bar{y}, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{3}^+$ $0, 0, z$ [001]	$y, y-x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{3}^-$ $0, 0, z$ [001]	$x-y, x, \bar{z}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
m $x, y, 0$ [001]	$x, y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{6}^+$ $0, 0, z$ [001]	$y-x, \bar{x}, \bar{z}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{6}^-$ $0, 0, z$ [001]	$\bar{y}, x-y, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
m $x, \bar{x}, z$ [110]	$\bar{y}, \bar{x}, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $x, 2x, z$ [100]	$y-x, y, z$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $2x, x, z$ [010]	$x, x-y, z$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$
m x, x, z [1$\bar{1}$0]	y, x, z	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $x, 0, z$ [120]	$x-y, \bar{y}, z$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $0, y, z$ [210]	$\bar{x}, y-x, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

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

and the translation part $\boldsymbol{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/4 \end{pmatrix}$. The assignment of the coordinate triplet to the matrix–column pair becomes obvious if one applies the equations (1.2.2.2) for the specific case of $(\boldsymbol{W}, \boldsymbol{w})$:

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ 1/4 \end{pmatrix}$$

would be

$$\tilde{x} = 0x + 1y + 0z + 1/2, \quad \tilde{y} = -1x + 0y + 0z + 1/2,$$
$$\tilde{z} = 0x + 0y + 1z + 1/4.$$

This symmetry operation is found under space group $P4_32_12$, No. 96 in the space-group tables of Chapter 2.3. It is the entry (4) of the first block (the so-called *General position* block) starting with 8 *b* 1 under the heading **Positions**.

(2) The matrix–column pair

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

is represented in shorthand notation by the coordinate triplet $\bar{x} + y, y, \bar{z} + 1/2$. This is the entry (11) of the general positions of the space group $P6_522$, No. 179 (*cf.* the space-group tables of Chapter 2.3).

1.2.2.2. Combination of mappings and inverse mappings

The combination of two symmetry operations $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ is again a symmetry operation. The linear and translation part of the combined symmetry operation is derived from the rotation and translation parts of $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ in a straightforward way:

Applying first the symmetry operation $(\boldsymbol{W}_1, \boldsymbol{w}_1)$, on the one hand,

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1,$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_2(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1) + \boldsymbol{w}_2 = \boldsymbol{W}_2\boldsymbol{W}_1\,\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2. \quad (1.2.2.5)$$

On the other hand

$$\tilde{\tilde{\boldsymbol{x}}} = (\boldsymbol{W}_2, \boldsymbol{w}_2)\tilde{\boldsymbol{x}} = (\boldsymbol{W}_2, \boldsymbol{w}_2)(\boldsymbol{W}_1, \boldsymbol{w}_1)\boldsymbol{x}. \quad (1.2.2.6)$$

By comparing equations (1.2.2.5) and (1.2.2.6) one obtains

$$(\boldsymbol{W}_2, \boldsymbol{w}_2)(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1, \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2). \quad (1.2.2.7)$$

The formula for the inverse of an affine mapping follows from the equations $\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, *i.e.* $\boldsymbol{x} = \boldsymbol{W}^{-1}\tilde{\boldsymbol{x}} - \boldsymbol{W}^{-1}\boldsymbol{w}$, which compared with $\boldsymbol{x} = (\boldsymbol{W}, \boldsymbol{w})^{-1}\tilde{\boldsymbol{x}}$ gives

$$(\boldsymbol{W}, \boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1}, -\boldsymbol{W}^{-1}\boldsymbol{w}). \quad (1.2.2.8)$$

Because of the inconvenience of these relations, especially for the column parts of the isometries, it is often preferable to use so-called *augmented matrices*, by which one can describe the combination of affine mappings and the inverse mapping by equations of matrix multiplication. These matrices are introduced in the following section.

1.2.2.3. Matrix–column pairs and (3 + 1) × (3 + 1) matrices

It is natural to combine the matrix part and the column part describing an affine mapping to form a (3 × 4) matrix, but such matrices cannot be multiplied by the usual matrix multiplication and cannot be inverted. However, if one supplements the (3 × 4) matrix by a fourth row '0 0 0 1', one obtains a (4 × 4) square matrix which can be combined with the analogous matrices of other mappings and can be inverted. These matrices are called *augmented matrices*, and here they are designated by open-face letters. Similarly, the columns $\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}$ also have to be extended to the augmented columns $\mathbb{x}$ and $\tilde{\mathbb{x}}$:

$$\mathbb{W} = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \quad \tilde{\mathbb{x}} = \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right), \quad \mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right). \qquad (1.2.2.9)$$

The horizontal and vertical lines in the augmented matrices are useful to facilitate recognition of their coefficients; they have no mathematical meaning.

Equations (1.2.2.1), (1.2.2.7) and (1.2.2.8) then become

$$\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}, \qquad (1.2.2.10)$$

$$\mathbb{W}_3 = \mathbb{W}_2\mathbb{W}_1 \text{ and } (\mathbb{W})^{-1} = (\mathbb{W}^{-1}). \qquad (1.2.2.11)$$

In the usual description by columns, the vector coefficients cannot be distinguished from the point coordinates, but in the augmented-column description the difference becomes visible.

If $\mathbb{p}$ and $\mathbb{q}$ are the augmented columns of coordinates of the points P and Q, $\mathbb{p} = \left(\begin{array}{c} p_1 \\ p_2 \\ p_3 \\ \hline 1 \end{array}\right)$ and $\mathbb{q} = \left(\begin{array}{c} q_1 \\ q_2 \\ q_3 \\ \hline 1 \end{array}\right)$, then $\mathbb{v} = \left(\begin{array}{c} q_1 - p_1 \\ q_2 - p_2 \\ q_3 - p_3 \\ \hline 0 \end{array}\right)$ is the augmented column $\mathbb{v}$ of the coefficients of the vector $\mathbf{v}$ between P and Q. The last coefficient of $\mathbb{v}$ is zero, because 1 − 1 = 0. Thus, the column of the coefficients of a vector is not augmented by '1' but by '0'. From the equation for the transformation of the vector coefficients $\tilde{\mathbb{v}} = \mathbb{W}\mathbb{v}$ it becomes clear that when the point P is mapped onto the point $\tilde{P}$ by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ according to equation (1.2.2.3), then the vector $\mathbf{v} = \overrightarrow{PQ}$ is mapped onto the vector $\tilde{\mathbf{v}} = \overrightarrow{\tilde{P}\tilde{Q}}$ by transforming its coefficients by $\tilde{\boldsymbol{v}} = \boldsymbol{W}\boldsymbol{v}$. This is because the coefficients w_j are multiplied by the number '0' augmenting the column $\boldsymbol{v} = (v_j)$. Indeed, the vector $\mathbf{v} = \overrightarrow{PQ}$ is not changed when the whole space is mapped onto itself by a translation.

1.2.2.4. The geometric meaning of (*W*, *w*)

Given the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ of a symmetry operation W, the geometric interpretation of W, *i.e.* the type of operation, screw or glide component, location *etc.*, can be calculated provided the coordinate system to which $(\boldsymbol{W}, \boldsymbol{w})$ refers is known.

(1) Evaluation of the matrix part $\boldsymbol{W}$:

(*a*) *Type of operation*: In general the coefficients of the matrix depend on the choice of the basis; a change of basis changes the coefficients, see Section 1.5.2. However, there are geometric quantities that are independent of the basis.

(i) The preservation of the handedness of a chiral object, *i.e.* the question of whether the symmetry operation is a rotation or rotoinversion, is a geometric property which is deduced from the determinant of $\boldsymbol{W}$: $\det(\boldsymbol{W}) = +1$: *rotation*; $\det(\boldsymbol{W}) = -1$: *rotoinversion*.

(ii) The *angle of rotation* ϕ. This does not depend on the coordinate basis. The corresponding invariant of the matrix $\boldsymbol{W}$ is the trace and it is defined by $tr(\boldsymbol{W}) = W_{11} + W_{22} + W_{33}$. The rotation angle ϕ of the rotation or of the rotation part of a rotoinversion can be calculated from the trace by the formula

$$\pm\mathrm{tr}(\boldsymbol{W}) = 1 + 2\cos\phi \quad \text{or} \quad \cos\phi = (\pm\mathrm{tr}(\boldsymbol{W}) - 1)/2. \qquad (1.2.2.12)$$

The + sign is used for rotations, the − sign for rotoinversions.

The type of isometry: the types 1, 2, 3, 4, 6 or $\bar{1}$, $\bar{2} = m$, $\bar{3}$, $\bar{4}$, $\bar{6}$ can be uniquely specified by the matrix invariants: the determinant $\det(\boldsymbol{W})$ and the trace $\mathrm{tr}(\boldsymbol{W})$:

	$\det(\boldsymbol{W}) = +1$					$\det(\boldsymbol{W}) = -1$				
$\mathrm{tr}(\boldsymbol{W})$	3	2	1	0	−1	−3	−2	−1	0	1
Type	1	6	4	3	2	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	$\bar{2} = m$
Order	1	6	4	3	2	2	6	4	6	2

(*b*) *Rotation or rotoinversion axis*: All symmetry operations (except 1 and $\bar{1}$) have a characteristic axis (the *rotation* or *rotoinversion axis*). The direction $\boldsymbol{u}$ of this axis is invariant under the symmetry operation:

$$\pm\boldsymbol{W}\boldsymbol{u} = \boldsymbol{u} \quad \text{or} \quad (\pm\boldsymbol{W} - \boldsymbol{I})\boldsymbol{u} = \boldsymbol{o}. \qquad (1.2.2.13)$$

The + sign is for rotations, the − sign for rotoinversions.

In the case of a k-fold rotation, the direction $\boldsymbol{u}$ can be calculated by the equation

$$\boldsymbol{u} = \boldsymbol{Y}(\boldsymbol{W})\boldsymbol{v} = (\boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{v}, \qquad (1.2.2.14)$$

where $\boldsymbol{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$ is an arbitrary direction. The direction $\boldsymbol{Y}(\boldsymbol{W})\boldsymbol{v}$ is invariant under the symmetry operation $\boldsymbol{W}$ as the multiplication with $\boldsymbol{W}$ just permutes the terms of $\boldsymbol{Y}$. If the application of equation (1.2.2.14) results in $\boldsymbol{u} = \boldsymbol{o}$, then the direction $\boldsymbol{v}$ is perpendicular to $\boldsymbol{u}$ and another direction $\boldsymbol{v}$ has to be selected. In the case of a rotoinversion $\boldsymbol{W}$, the direction $\boldsymbol{Y}(-\boldsymbol{W})\boldsymbol{v}$ gives the direction of the rotoinversion axis. For $\bar{2} = m$, $\boldsymbol{Y}(-\boldsymbol{W}) = -\boldsymbol{W} + \boldsymbol{I}$.

(*c*) *Sense of rotation* (for rotations or rotoinversions with $k > 2$): The sense of rotation is determined by the sign of the determinant of the matrix $\boldsymbol{Z}$, given by $\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\boldsymbol{W}\boldsymbol{x}]$, where $\boldsymbol{u}$ is the vector of equation (1.2.2.14) and $\boldsymbol{x}$ is a non-parallel vector of $\boldsymbol{u}$, *e.g.* one of the basis vectors.

Examples are given later.

(2) Analysis of the translation column $\boldsymbol{w}$:

(*a*) If $\boldsymbol{W}$ is the matrix of a rotation of order k or of a reflection ($k = 2$), then $\boldsymbol{W}^k = \boldsymbol{I}$, and one determines the *intrinsic translation part* (or *screw part* or *glide part*) of the symmetry operation, also called the *intrinsic translation component* of the symmetry operation, $\boldsymbol{w}_g = \boldsymbol{t}/k$ by

$$(\boldsymbol{W},\boldsymbol{w})^k = (\boldsymbol{W}^k, \boldsymbol{W}^{k-1}\boldsymbol{w} + \boldsymbol{W}^{k-2}\boldsymbol{w} + \ldots + \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{t}) \quad (1.2.2.15)$$

or

$$\boldsymbol{w}_g = \boldsymbol{t}/k = \frac{1}{k}(\boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} = \frac{1}{k}\boldsymbol{Y}(\boldsymbol{W})\,\boldsymbol{w}. \quad (1.2.2.16)$$

The vector with the column of coefficients $\boldsymbol{w}_g = \boldsymbol{t}/k$ is called the *screw* or *glide vector*. This vector is invariant under the symmetry operation: $\boldsymbol{W}\boldsymbol{w}_g = \boldsymbol{w}_g$. Indeed, multiplication with $\boldsymbol{W}$ permutes only the terms on the right side of equation (1.2.2.16). Thus, the screw vector of a screw rotation is parallel to the screw axis. The glide vector of a glide reflection is left invariant for the same reason. It is parallel to the glide plane because $(-\boldsymbol{W} + \boldsymbol{I})(\boldsymbol{I} + \boldsymbol{W}) = \boldsymbol{O}$.

If $\boldsymbol{t} = \boldsymbol{o}$ holds, then $(\boldsymbol{W}, \boldsymbol{w})$ describes a *rotation* or *reflection*. For $\boldsymbol{t} \neq \boldsymbol{o}$, $(\boldsymbol{W}, \boldsymbol{w})$ describes a *screw rotation* or *glide reflection*. One forms the so-called *reduced operation* by subtracting the *intrinsic translation part* $\boldsymbol{w}_g = \boldsymbol{t}/k$ from $(\boldsymbol{W}, \boldsymbol{w})$:

$$(\boldsymbol{I}, -\boldsymbol{t}/k)(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} - \boldsymbol{w}_g) = (\boldsymbol{W}, \boldsymbol{w}_l). \quad (1.2.2.17)$$

The column $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{t}/k$ is called the *location part* (or the *location component* of the translation part) of the symmetry operation because it determines the position of the rotation or screw–rotation axis or of the reflection or glide–reflection plane in space.

(*b*) The set of *fixed points* of a symmetry operation is obtained by solving the equation

$$\boldsymbol{W}\boldsymbol{x}_F + \boldsymbol{w} = \boldsymbol{x}_F. \quad (1.2.2.18)$$

Equation (1.2.2.18) has a unique solution for all rotoinversions (including $\bar{1}$, excluding $\bar{2} = m$). There is a one-dimensional set of solutions for rotations (the rotation axis) and a two-dimensional set of solutions for reflections (the mirror plane). For translations, screw rotations and glide reflections, there are no solutions: there are no fixed points. However, a solution is found for the reduced operation, *i.e.* after subtraction of the intrinsic translation part, *cf.* equation (1.2.2.17)

$$\boldsymbol{W}\boldsymbol{x}_F + \boldsymbol{w}_l = \boldsymbol{x}_F. \quad (1.2.2.19)$$

(Note that the reduced operation of a translation is the identity, whose set of fixed points is the whole space.)

The formulae of this section enable the user to find the geometric contents of any symmetry operation. In practice, the geometric meanings for all symmetry operations which are listed in the *General position* blocks of the space-group tables of Part 2 can be found in the corresponding **Symmetry operations** blocks of the space-group tables. The explanation of the symbols for the symmetry operations is found in Sections 1.4.2 and 2.1.3.9.

The procedure for the geometric interpretation of the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ of the symmetry operations is illustrated by three examples of the space group $Ia\bar{3}d$, No. 230 (*cf.* the space-group tables of Chapter 2.3).

Examples

(1) Consider the symmetry operation $y + \frac{1}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$ [symmetry operation (15) of the *General position* (0, 0, 0) block of the space group $Ia\bar{3}d$]. Its matrix–column pair is given by

$$\boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \boldsymbol{w} = \begin{pmatrix} 1/4 \\ 1/4 \\ 3/4 \end{pmatrix}.$$

Type of operation: the values of det($\boldsymbol{W}$) = 1 and tr($\boldsymbol{W}$) = 1 show that the symmetry operation is a fourfold rotation.
The direction of rotation axis $\boldsymbol{u}$: The application of equation (1.2.2.14) with the matrix

$$\boldsymbol{Y}(\boldsymbol{W}) = (\boldsymbol{W}^3 + \boldsymbol{W}^2 + \boldsymbol{W} + \boldsymbol{I}) = (\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

yields the direction $\boldsymbol{u}$ = [001] of the fourfold rotation axis.
Sense of rotation: The negative sense of rotation follows from det($\boldsymbol{Z}$) = −1, where the matrix

$$\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\boldsymbol{W}\boldsymbol{x}] = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$$

(here, $\boldsymbol{x} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ is taken as a vector non-parallel to $\boldsymbol{u}$).
Screw component: The intrinsic translation part (screw component) $\boldsymbol{w}_g$ of the symmetry operation is calculated from

$$\boldsymbol{w}_g = \tfrac{1}{4}\boldsymbol{Y}(\boldsymbol{W})\boldsymbol{w} = 1/4\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}\begin{pmatrix} 1/4 \\ 1/4 \\ 3/4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 3/4 \end{pmatrix}.$$

Location of the symmetry operation: The location of the fourfold screw rotation is given by the fixed points of the reduced symmetry operation $(\boldsymbol{W}, \boldsymbol{w} - \boldsymbol{w}_g)$. The set of fixed points $\boldsymbol{x}_F = \begin{pmatrix} 1/4 \\ 0 \\ z \end{pmatrix}$ is obtained from the equation

$$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} + \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}.$$

Following the conventions for the designation of symmetry operations adopted in this volume (*cf.* Section 1.4.2 and 2.1.3.9), the symbol of the symmetry operation $y + \frac{1}{4}$, $-x + \frac{1}{4}$, $z + \frac{3}{4}$ is given by $4^-(0, 0, \frac{3}{4})$ $\frac{1}{4}, 0, z$.

(2) The symmetry operation $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y$ with

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

corresponds to the entry No. (30) of the *General position* (0, 0, 0) block of the space group $Ia\bar{3}d$, No. 230.

Type of operation: the values of $\det(\boldsymbol{W}) = -1$ and $\mathrm{tr}(\boldsymbol{W}) = 0$ show that symmetry operation is a threefold rotoinversion.

The direction of rotoinversion axis $\boldsymbol{u}$:

$$\boldsymbol{Y}(-\boldsymbol{W}) = (\boldsymbol{W}^2 - \boldsymbol{W} + \boldsymbol{I}) = \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right) = \begin{pmatrix} 1 & \bar{1} & 1 \\ \bar{1} & 1 & \bar{1} \\ 1 & \bar{1} & 1 \end{pmatrix}$$

yields the direction $\boldsymbol{u} = [\bar{1}1\bar{1}]$ from $\boldsymbol{v} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$.

Sense of rotation: The positive sense of rotation follows from the positive sign of the determinant of the matrix $\boldsymbol{Z}$, $\det(\boldsymbol{Z}) = 1$, where the matrix

$$\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\boldsymbol{W}\boldsymbol{x}] = \begin{pmatrix} \bar{1} & 0 & 1 \\ 1 & 0 & 0 \\ \bar{1} & 1 & 0 \end{pmatrix}$$

(here, $\boldsymbol{x} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ is taken as a vector non-parallel to $\boldsymbol{u}$).

Location of the symmetry operation: The solution $x_F = 0$, $y_F = 1/2, z_F = 1/2$ of the fixed-point equation of the rotoinversion

$$\begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}$$

gives the coordinates of the inversion centre on the rotoinversion axis. An obvious description of a line along the direction $\boldsymbol{u} = [\bar{1}1\bar{1}]$ and passing through the point $(0, 1/2, 1/2)$ is given by the parametric expression $\bar{u}, u + 1/2, \bar{u} + 1/2$. The choice of the free parameter $u = x + 1/2$ results in the description $\bar{x} - 1/2, x + 1, \bar{x}$ of the rotoinversion axis found in the **Symmetry operation** (0, 0, 0) block. The convention adopted in this volume to have zero constant at the z coordinate of the description of the $\bar{3}$ axis determines the specific choice of the free parameter.

The geometric characteristics of the symmetry operation $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y$ are reflected in its symbol $\bar{3}^+\ \bar{x} - 1/2, x + 1, \bar{x};\ 0, \frac{1}{2}, \frac{1}{2}$.

(3) The matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ of the symmetry operation (37) $\bar{y} + 3/4, \bar{x} + 1/4, z + 1/4$ of the *General position* (1/2, 1/2, 1/2) block of the space group $Ia\bar{3}d$ is given by

$$\boldsymbol{W} = \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \boldsymbol{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}.$$

Type of operation: The values of the determinant $\det(\boldsymbol{W}) = -1$ and the trace $\mathrm{tr}(\boldsymbol{W}) = +1$ indicate that the symmetry operation is a reflection.

Normal $\boldsymbol{u}$ *of the reflection plane*: The orientation of the reflection plane in space is determined by its normal $\boldsymbol{u}$, which is directed along [110]. The direction of $\boldsymbol{u}$ follows from the matrix equation

$$\boldsymbol{u} = (-\boldsymbol{W} + \boldsymbol{I})\boldsymbol{v} = \left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)\boldsymbol{v} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\boldsymbol{v},$$

where $\boldsymbol{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$ is arbitrary.

Glide component: The glide component $\boldsymbol{w}_g = \begin{pmatrix} 1/4 \\ -1/4 \\ 1/4 \end{pmatrix}$, determined from the equation

$$\boldsymbol{w}_g = \tfrac{1}{2}(\boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} = \tfrac{1}{2}\left(\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)\begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix},$$

indicates that the symmetry operation is a d-glide reflection. As expected, the translation vector

$$\mathbf{t} = 2\boldsymbol{w}_g = \begin{pmatrix} 1/2 \\ -1/2 \\ 1/2 \end{pmatrix}$$

corresponds to a centring translation.

Location of the symmetry operation: The location of the d-glide plane follows from the set of fixed points (x_F, y_F, z_F) of the reduced symmetry operation

$$(\boldsymbol{W}, \boldsymbol{w} - \boldsymbol{w}_g) = \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 3/4 - 1/4 \\ 1/4 - (-1/4) \\ 1/4 - 1/4 \end{pmatrix}\right):$$

$$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}.$$

Thus, the set of fixed points (the d-glide plane) can be described as $x + 1/2, \bar{x}, z$.

The symbol $d\,(1/4, -1/4, 1/4)\ x + 1/2, \bar{x}, z$ of the symmetry operation (37) $\bar{y} + 3/4, \bar{x} + 1/4, z + 1/4$, found in the **Symmetry operations** (1/2, 1/2, 1/2) block of the space-group table of $Ia\bar{3}d$ in Chapter 2.3, comprises the essential geometric characteristics of the symmetry operation, *i.e.* its type, glide component and location. It is worth repeating that according to the conventions adopted in the space-group tables of Part 2, the mirror planes are specified by their sets of fixed points and not by the normals to the planes (*cf.* Section 1.4.2 for more details).

1.2.2.5. Determination of matrix–column pairs of symmetry operations

The specification of the symmetry operations by their types, screw or glide components and locations is sufficient to determine the corresponding matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$. The general idea is to determine the image points $\tilde{X}$ of some points X under the symmetry operation by applying geometrical considerations. The 12 unknown coefficients of $(\boldsymbol{W}, \boldsymbol{w})$ (nine coefficients W_{ik} and three coefficients w_j) can then be calculated as solutions of 12 inhomogeneous linear equations obtained from the system of 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

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

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

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

[*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

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

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; $2\mathbf{v}$ (not $\mathbf{v}$) 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 **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 **u**.

(*a*) Twofold screw axis ∥ [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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