International Tables for Crystallography (2016). Vol. A, Section 1.2.1, pp. 12–13.

1.2. Crystallographic symmetry

H. Wondratschek and M. I. Aroyo

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* $\mathbf{w}_g$ 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

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

The symbols $(\boldsymbol{W}, \boldsymbol{w})$ and $\{\boldsymbol{W} \mid \boldsymbol{w}\}$ 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.

references