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11.1. Point coordinates, symmetry operations and their symbols

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11.1.1. Coordinate triplets and symmetry operations

The coordinate triplets of a general position, as given in the space-group tables, can be taken as a shorthand notation for the symmetry operations of the space group. Each coordinate triplet $\tilde{x}, \tilde{y}, \tilde{z}$ corresponds to the symmetry operation that maps a point with coordinates x, y, z onto a point with coordinates $\tilde{x}, \tilde{y}, \tilde{z}$. The mapping of x, y, z onto $\tilde{x}, \tilde{y}, \tilde{z}$ is given by the equations:

$$\tilde{x} = W_{11}x + W_{12}y + W_{13}z + w_1$$
$$\tilde{y} = W_{21}x + W_{22}y + W_{23}z + w_2$$
$$\tilde{z} = W_{31}x + W_{32}y + W_{33}z + w_3.$$

If, as usual, the symmetry operation is represented by a matrix pair, consisting of a (3×3) matrix $\boldsymbol{W}$ and a (3×1) column matrix $\boldsymbol{w}$, the equations read

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

with

$$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \tilde{\boldsymbol{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix},$$

$$\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}, \quad \boldsymbol{W} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix}.$$

$\boldsymbol{W}$ is called the rotation part and $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$ the translation part; $\boldsymbol{w}$ is the sum of the intrinsic translation part $\boldsymbol{w}_g$ (glide part or screw part) and the location part $\boldsymbol{w}_l$ (due to the location of the symmetry element) of the symmetry operation.

Example

The coordinate triplet $-x + y, y, -z + \frac{1}{2}$ stands for the symmetry operation with rotation part

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

and with translation part

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

Matrix multiplication yields

$$\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -x + y \\ y \\ -z + \frac{1}{2} \end{pmatrix}.$$

Using the above relation, the assignment of coordinate triplets to symmetry operations given as pairs $(\boldsymbol{W}, \boldsymbol{w})$ is straightforward.

11.1.2. Symbols for symmetry operations

The information required to describe a symmetry operation by a unique notation depends on the type of the operation (Table 11.1.2.1). The symbols explained below are based on the Hermann–Mauguin symbols (see Chapter 12.2), modified and supplemented where necessary. Note that a change of the coordinate basis generally alters the symbol of a given symmetry operation.

(i) A *translation* is symbolized by the letter *t,* followed by the components of the translation vector between parentheses.

Example

$t(\frac{1}{2}, \frac{1}{2}, 0)$ stands for a translation by the vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, *i.e.* a *C* centring.

(ii) A *rotation* is symbolized by a number $n = 2$, 3, 4 or 6 (according to the rotation angle $360°/n$) and a superscript, + or −, which specifies the sense of rotation (not needed for $n = 2$). This is followed by the location of the rotation axis. Since the definition of the positive sense of a pure rotation is arbitrary, the following convention has been adopted: The sense of a rotation is symbolized by + if the rotation appears to be in the mathematically positive sense (*i.e.* counter-clockwise) when viewed along the rotation axis in the direction of decreasing values of the parameter describing that axis. This convention leads to a particular symbol for each rotation and avoids describing some rotations by powers of other rotations. It corresponds to looking at the usual tetragonal or hexagonal space-group diagrams.

Example

$4^+ \; 0, y, 0$ indicates a rotation of 90° about the line $0y0$ that brings point 001 onto point 100, a rotation that is seen in the mathematically positive sense if viewed from point 010 to point 000.

(iii) A *screw rotation* is symbolized in the same way as a pure rotation, but with the screw part added between parentheses.

Example

$3^- \; (0, 0, \frac{1}{3}) \; \frac{1}{3}, \frac{1}{3}, z$ indicates a rotation of 120° around the line $\frac{1}{3}\frac{1}{3}z$ in the mathematically negative sense if viewed from the point $\frac{1}{3}\frac{1}{3}1$ towards $\frac{1}{3}\frac{1}{3}0$, combined with a translation of $\frac{1}{3}\mathbf{c}$.

Thus, with respect to the coordinate basis chosen, each screw rotation is designated uniquely. This could not have been achieved by deriving the screw-rotation symbols from the Hermann–Mauguin screw-axis symbols.

Table 11.1.2.1. *Information necessary to describe symmetry operations*

Type of symmetry operation	Necessary information
Translation	Translation vector
Rotation	Location of the rotation axis, angle and sense of rotation
Screw rotation	As for rotation, plus screw vector
Reflection	Location of the mirror plane
Glide reflection	As for reflection, plus glide vector
Inversion	Location of the inversion centre
Rotoinversion	As for rotation, plus location of the inversion point

Example

The symmetry operation represented by $-y, z+\frac{1}{2}, -x+\frac{1}{2}$ occurs in space group $P2_13$ as well as in $I2_13$ and is labelled (10) in the space-group tables (see Section 2.2.9) both times. The corresponding symmetry element, however, is a 3_1 axis in $P2_13$, but a 3_2 axis in $I2_13$, because the subscript refers to the shortest translation parallel to the axis.

(iv) A *reflection* is symbolized by the letter m, followed by the location of the mirror plane.

(v) A *glide reflection* in general is symbolized by the letter g, with the glide part given between parentheses, followed by the location of the glide plane. These specifications characterize every glide reflection uniquely. Exceptions are the traditional symbols a, b, c, n and d that are used instead of g. In the case of a glide plane a, b or c, the explicit statement of the glide vector is omitted if it is $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$ or $\frac{1}{2}\mathbf{c}$, respectively.

Example

$a\ x, y, \frac{1}{4}$ means a glide reflection with glide part $\frac{1}{2}\mathbf{a}$ and the glide plane a at $x\,y\,\frac{1}{4}$; $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})\ x, x-\frac{1}{4}, z$ denotes a glide reflection with glide part $(\frac{1}{4}\frac{1}{4}\frac{3}{4})$ and the glide plane d at $x, x-\frac{1}{4}, z$.

The letter g is kept for those glide reflections that cannot be described with one of the symbols a, b, c, n, d without additional conventions.

Example

$g(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})\ x+\frac{1}{2}, -x, z$ implies a glide reflection with glide part $(-\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$ and the glide plane at $x+\frac{1}{2}, -x, z$.

(vi) An *inversion* is symbolized by $\overline{1}$, followed by the location of the symmetry centre.

(vii) A *rotoinversion* is symbolized, in analogy to a rotation, by $\overline{3}, \overline{4}$ or $\overline{6}$ and the superscript $+$ or $-$, again followed by the location of the (rotoinversion) axis. Note that angle and sense of rotation refer to the pure rotation and not to the combination of rotation and inversion. In addition, the location of the inversion point is given by the appropriate coordinate triplet after a semicolon.

Example

$\overline{4}^{+}\ 0, \frac{1}{2}, z;\ 0, \frac{1}{2}, \frac{1}{4}$ means a 90° rotoinversion with axis at $0\frac{1}{2}z$ and inversion point at $0\frac{1}{2}\frac{1}{4}$. The rotation is performed in the mathematically positive sense, when viewed from $0\frac{1}{2}1$ towards $0\frac{1}{2}0$. Therefore, the rotoinversion maps point 000 onto point $-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

references