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5.1. Transformations of the coordinate system (unit-cell transformations)

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5.1.1. Introduction

There are two main uses of transformations in crystallography.

(i) *Transformation of the coordinate system* and the unit cell while keeping the crystal at rest. This aspect forms the main topic of the present part. Transformations of coordinate systems are useful when nonconventional descriptions of a crystal structure are considered, for instance in the study of relations between different structures, of phase transitions and of group–subgroup relations. Unit-cell transformations occur particularly frequently when different settings or cell choices of monoclinic, orthorhombic or rhombohedral space groups are to be compared or when 'reduced cells' are derived.

(ii) Description of the *symmetry operations* (motions) of an object (crystal structure). This involves the transformation of the coordinates of a point or the components of a position vector while keeping the coordinate system unchanged. Symmetry operations are treated in Chapter 8.1 and Part 11. They are briefly reviewed in Chapter 5.2.

5.1.2. Matrix notation

Throughout this volume, matrices are written in the following notation:

As (1 × 3) row matrices:

$(\mathbf{a}, \mathbf{b}, \mathbf{c})$	the basis vectors of direct space
(h, k, l)	the Miller indices of a plane (or a set of planes) in direct space or the coordinates of a point in reciprocal space

As (3 × 1) or (4 × 1) column matrices:

$x = (x/y/z)$	the coordinates of a point in direct space
$(\mathbf{a}^*/\mathbf{b}^*/\mathbf{c}^*)$	the basis vectors of reciprocal space
$(u/v/w)$	the indices of a direction in direct space
$\boldsymbol{p} = (p_1/p_2/p_3)$	the components of a shift vector from origin O to the new origin O'
$\boldsymbol{q} = (q_1/q_2/q_3)$	the components of an inverse origin shift from origin O' to origin O, with $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$
$\boldsymbol{w} = (w_1/w_2/w_3)$	the translation part of a symmetry operation W in direct space
$\mathbb{X} = (x/y/z/1)$	the augmented (4×1) column matrix of the coordinates of a point in direct space

As (3 × 3) or (4 × 4) square matrices:

$\boldsymbol{P}, \boldsymbol{Q} = \boldsymbol{P}^{-1}$	linear parts of an affine transformation; if $\boldsymbol{P}$ is applied to a (1×3) row matrix, $\boldsymbol{Q}$ must be applied to a (3×1) column matrix, and *vice versa*
$\boldsymbol{W}$	the rotation part of a symmetry operation W in direct space
$\mathbb{P} = \begin{pmatrix} \boldsymbol{P} & \boldsymbol{p} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented affine (4×4) transformation matrix, with $\boldsymbol{o} = (0, 0, 0)$
$\mathbb{Q} = \begin{pmatrix} \boldsymbol{Q} & \boldsymbol{q} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented affine (4×4) transformation matrix, with $\mathbb{Q} = \mathbb{P}^{-1}$
$\mathbb{W} = \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented (4×4) matrix of a symmetry operation in direct space (*cf.* Chapter 8.1 and Part 11).

5.1.3. General transformation

Here the crystal structure is considered to be at rest, whereas the coordinate system and the unit cell are changed. Specifically, a point X in a crystal is defined with respect to the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and the origin O by the coordinates x, y, z, *i.e.* the position vector $\mathbf{r}$ of point X is given by

$$\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

The same point X is given with respect to a new coordinate system, *i.e.* the new basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ and the new origin O' (Fig. 5.1.3.1), by the position vector

$$\mathbf{r}' = x'\mathbf{a}' + y'\mathbf{b}' + z'\mathbf{c}'.$$

In this section, the relations between the primed and unprimed quantities are treated.

The general transformation (affine transformation) of the coordinate system consists of two parts, a linear part and a shift of origin. The (3×3) matrix $\boldsymbol{P}$ of the linear part and the (3×1) column matrix $\boldsymbol{p}$, containing the components of the shift vector $\boldsymbol{p}$, define the transformation uniquely. It is represented by the symbol $(\boldsymbol{P}, \boldsymbol{p})$.

(i) The *linear part* implies a change of orientation or length or both of the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$, *i.e.*

$$\begin{aligned}(\mathbf{a}', \mathbf{b}', \mathbf{c}') &= (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P} \\ &= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \\ &= (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \\ &\quad P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \\ &\quad P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}).\end{aligned}$$

For a pure linear transformation, the shift vector $\mathbf{p}$ is zero and the symbol is $(\boldsymbol{P}, \boldsymbol{o})$.

The determinant of $\boldsymbol{P}$, $\det(\boldsymbol{P})$, should be positive. If $\det(\boldsymbol{P})$ is negative, a right-handed coordinate system is transformed into a left-handed one (or *vice versa*). If $\det(\boldsymbol{P}) = 0$, the new basis vectors are linearly dependent and do not form a complete coordinate system.

In this chapter, transformations in three-dimensional space are treated. A change of the basis vectors in two dimensions, *i.e.* of the basis vectors $\mathbf{a}$ and $\mathbf{b}$, can be considered as a three-dimensional transformation with invariant $\mathbf{c}$ axis. This is achieved by setting $P_{33} = 1$ and $P_{13} = P_{23} = P_{31} = P_{32} = 0$.

(ii) A *shift of origin* is defined by the shift vector

$$\mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}.$$

The basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are fixed at the origin O; the new basis vectors are fixed at the new origin O' which has the coordinates p_1, p_2, p_3 in the old coordinate system (Fig. 5.1.3.1).

For a pure origin shift, the basis vectors do not change their lengths or orientations. In this case, the transformation matrix $\boldsymbol{P}$ is the unit matrix $\boldsymbol{I}$ and the symbol of the pure shift becomes $(\boldsymbol{I}, \boldsymbol{p})$.

references