distance vector $\mathbf{v} = \overrightarrow{PQ}$ is not changed when the whole space is mapped onto itself by a translation.

Remarks:

(1) The difference in transformation behaviour between the point coordinates $\boldsymbol{x}$ and the vector coefficients $\boldsymbol{v}$ is not visible in the equations where the symbols $\mathbb{x}$ and $\mathbb{v}$ are used, but is obvious only if the columns are written in full, *viz*

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \hline 1 \end{pmatrix} \text{ and } \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \hline 0 \end{pmatrix}.$$

(2) The transformation behaviour of the vector coefficients is also apparent if the vector is understood to be a translation vector and the transformation behaviour of the translation is considered as in the last paragraph of the next section.

(3) The transformation $\tilde{\boldsymbol{v}} = \boldsymbol{W}\boldsymbol{v}$ is called an *orthogonal mapping* if $\boldsymbol{W}$ is the matrix part of an isometry.

1.2.2.7. *Origin shift and change of the basis*

It is in general advantageous to refer crystallographic objects and their symmetries to the most appropriate coordinate system. The best coordinate system may be different for different steps of the calculations and for different objects which have to be considered simultaneously. Therefore, a change of the origin and/or the basis are frequently necessary when treating crystallographic problems. Here the formulae for the influence of an origin shift and a change of basis on the coordinates, on the matrix–column pairs of mappings and on the vector coefficients are only stated; the equations are derived in detail in *IT* A Chapters 5.2 and 5.3, and in Hahn & Wondratschek (1994).

Let a coordinate system be given with a basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\rm T}$ and an origin O.[1] Referred to this coordinate system, the column of coordinates of a point P is $\boldsymbol{x}$; the matrix and column parts describing a symmetry operation are $\boldsymbol{W}$ and $\boldsymbol{w}$ according to equations (1.2.2.1) to (1.2.2.3), and the column of vector coefficients is $\boldsymbol{v}$, see Section 1.2.2.6. A new coordinate system may be introduced with the basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\rm T}$ and the origin O'. Referred to the new coordinate system, the column of coordinates of the point P is $\boldsymbol{x}'$, the symmetry operation is described by $\boldsymbol{W}'$ and $\boldsymbol{w}'$ and the column of vector coefficients is $\boldsymbol{v}'$.

Let $\boldsymbol{p} = \overrightarrow{OO'}$ be the column of coefficients for the vector from the old origin O to the new origin O' and let

$$\boldsymbol{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \qquad (1.2.2.9)$$

be the matrix of a basis change, *i.e.* the matrix that relates the new basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\rm T}$ to the old basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\rm T}$ according to

$$(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\rm T} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\rm T}\boldsymbol{P} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\rm T}\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}. \qquad (1.2.2.10)$$

[1] In this volume, point coordinates and vector coefficients are thought of as columns in matrix multiplication. Therefore, columns are considered to be 'standard'. These 'columns' are not marked, even if they are written in a row. To comply with the rules of matrix multiplication, rows are also introduced. These rows of symbols (*e.g.* vector coefficients of reciprocal space, *i.e.* Miller indices, or a set of basis vectors of direct space) are 'transposed relative to columns' and are, therefore, marked $(h, k, l)^{\rm T}$ or $(\mathbf{a}, \mathbf{b}, \mathbf{c})^{\rm T}$, even if they are written in a row.

Then the following equations hold:

$$\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} - \boldsymbol{P}^{-1}\boldsymbol{p} \ \text{ or } \ \boldsymbol{x} = \boldsymbol{P}\boldsymbol{x}' + \boldsymbol{p}; \qquad (1.2.2.11)$$

$$\boldsymbol{W}' = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \ \text{ or } \ \boldsymbol{W} = \boldsymbol{P}\boldsymbol{W}'\boldsymbol{P}^{-1}; \qquad (1.2.2.12)$$

$$\boldsymbol{w}' = \boldsymbol{P}^{-1}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}) \ \text{ or } \ \boldsymbol{w} = \boldsymbol{P}\boldsymbol{w}' - (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}. \qquad (1.2.2.13)$$

For the columns of vector coefficients $\boldsymbol{v}$ and $\boldsymbol{v}'$, the following holds:

$$\boldsymbol{v}' = \boldsymbol{P}^{-1}\boldsymbol{v} \ \text{ or } \ \boldsymbol{v} = \boldsymbol{P}\boldsymbol{v}', \qquad (1.2.2.14)$$

i.e. an origin shift does not change the vector coefficients.

These equations read in the augmented-matrix formalism

$$\mathbb{x}' = \mathbb{P}^{-1}\mathbb{x}; \ \mathbb{W}' = \mathbb{P}^{-1}\mathbb{W}\mathbb{P}; \ \mathbb{v}' = \mathbb{P}^{-1}\mathbb{v}. \qquad (1.2.2.15)$$

For the difference in the transformation behaviour of point coordinates and vector coefficients, see the remarks at the end of Section 1.2.2.6. A vector $\mathbf{v}$ can be regarded as a translation vector; its translation is then described by $(\boldsymbol{I}, \boldsymbol{v})$, *i.e.* $\boldsymbol{W} = \boldsymbol{I}$, $\boldsymbol{w} = \boldsymbol{v}$. It can be shown using equation (1.2.2.13) that the translation and thus the translation vector are not changed under an origin shift, $(\boldsymbol{I}, \boldsymbol{p})$, because $(\boldsymbol{I}, \boldsymbol{v})' = (\boldsymbol{I}, \boldsymbol{v})$ holds. Moreover, under a general coordinate transformation the origin shift is not effective: in equation (1.2.2.13) only $\boldsymbol{v}' = \boldsymbol{P}^{-1}\boldsymbol{v}$ remains because of the equality $\boldsymbol{W} = \boldsymbol{I}$.

1.2.3. Groups

Group theory is the proper tool for studying symmetry in science. The symmetry group of an object is the set of all isometries (rigid motions) which map that object onto itself. If the object is a crystal, the isometries which map it onto itself (and also leave it invariant as a whole) are the *crystallographic symmetry operations*.

There is a huge amount of literature on group theory and its applications. The book *Introduction to Group Theory* by Ledermann (1976) is recommended. The book *Symmetry of Crystals. Introduction to International Tables for Crystallography, Vol. A* by Hahn & Wondratschek (1994) describes a way in which the data of *IT* A can be interpreted by means of matrix algebra and elementary group theory. It may also help the reader of this volume.

1.2.3.1. *Some properties of symmetry groups*

The geometric symmetry of any object is described by a group $\mathcal{G}$. The symmetry operations $g_j \in \mathcal{G}$ are the group elements, and the set $\{g_j \in \mathcal{G}\}$ of all symmetry operations fulfils the group postulates. [A 'symmetry element' in crystallography is not a group element of a symmetry group but is a combination of a geometric object with that set of symmetry operations which leave the geometric object invariant, *e.g.* an axis with its threefold rotations or a plane with its glide reflections *etc.*, *cf.* Flack *et al.* (2000).] Groups will be designated by upper-case calligraphic script letters $\mathcal{G}$, $\mathcal{H}$ *etc*. Group elements are represented by lower-case slanting *sans serif* letters g, h *etc.*

The result g_r of the composition of two elements g_j, $g_k \in \mathcal{G}$ will be called the *product* of g_j and g_k and will be written $g_r = g_k\, g_j$. The first operation is the right factor because the point coordinates or vector coefficients are written as columns on which the matrices of the symmetry operations are applied from the left side.

The *law of composition* in the group is the successive application of the symmetry operations.

The *group postulates* are shown to hold for symmetry groups:

(1) The *closure*, *i.e.* the property that the composition of any two symmetry operations results in a symmetry operation again, is always fulfilled for geometric symmetries: if $g_j \in \mathcal{G}$ and $g_k \in \mathcal{G}$, then $g_j\, g_k = g_r \in \mathcal{G}$ also holds.