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1.2. General introduction to the subgroups of space groups

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1.2.1. General remarks

The performance of simple vector and matrix calculations, as well as elementary operations with groups, are nowadays common practice in crystallography, especially since computers and suitable programs have become widely available. The authors of this volume therefore assume that the reader has at least some practical experience with matrices and groups and their crystallographic applications. The explanations and definitions of the basic terms of linear algebra and group theory in these first sections of this introduction are accordingly short. Rather than replace an elementary textbook, these first sections aim to acquaint the reader with the method of presentation and the terminology that the authors have chosen for the tables and graphs of this volume. The concepts of groups, their subgroups, isomorphism, coset decomposition and conjugacy are considered to be essential for the use of the tables and for their practical application to crystal structures; for a deeper understanding the concept of normalizers is also necessary. Frequently, however, an 'intuitive feeling' obtained by practical experience may replace a full comprehension of the mathematical meaning. From Section 1.2.6 onwards, the presentation will be more detailed because the subjects are more specialized (but mostly not more difficult) and are seldom found in textbooks.

1.2.2. Mappings and matrices

1.2.2.1. Crystallographic symmetry operations

A crystal is a finite block of an infinite periodic array of atoms in physical space. The infinite periodic array is called the *crystal pattern*. The finite block is called the *macroscopic crystal*.[1]

Periodicity implies that there are *translations* which map the crystal pattern onto itself. 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*. The mapping is *reversible* if each image point $\tilde{P}$ is the image of one point P only.

Translations belong to a special category of mappings which leave all distances in the space invariant (and thus within an object and between objects in the space). Furthermore, a mapping of an object onto itself (German: *Deckoperation*) is the basis of the concept of geometric symmetry. This is expressed by the following two definitions.

Definition 1.2.2.1.1. 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. □

An isometry is a special kind of affine mapping. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but quotients of lengths on the same line are preserved. In Section 1.2.2.3, the description of affine mappings is discussed, because this type of description also applies to isometries. Affine mappings are important for the classification of crystallographic symmetries, *cf.* Section 1.2.5.2.

Definition 1.2.2.1.2. A mapping is called a *symmetry operation* of an object if

(1) it is an isometry,
(2) it maps the object onto itself. □

Instead of 'maps the object onto itself', one frequently says 'leaves the object invariant (as a whole)'. This does not mean that each point of the object is mapped onto itself; rather, the object is mapped in such a way that an observer cannot distinguish the states of the object before and after the mapping.

Definition 1.2.2.1.3. A symmetry operation of a crystal pattern is called a *crystallographic symmetry operation*. □

The symmetry operations of a macroscopic crystal are also crystallographic symmetry operations, but they belong to another kind of mapping which will be discussed in Section 1.2.5.4.

There are different types of isometries which may be crystallographic symmetry operations. These types are described and discussed in many textbooks of crystallography and in mathematical, physical and chemical textbooks. They are listed here without further treatment. Fixed points are very important for the characterization of isometries.

Definition 1.2.2.1.4. 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).

The following kinds of isometries exist:

(1) The *identity operation*, which maps each point of the space onto itself. It is a symmetry operation of every object and, although trivial, is indispensable for the group properties which are discussed in Section 1.2.3.
(2) A *translation* t which shifts every object. A translation is characterized by its translation vector $\mathbf{t}$ and has no fixed point: if $\boldsymbol{x}$ is the column of coordinates of a point P, then the coordinates $\tilde{x}$ of the image point $\tilde{P}$ are $\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{t}$. If a translation is a symmetry operation of an object, the object extends infinitely in the directions of $\mathbf{t}$ and $-\mathbf{t}$. A translation preserves the 'handedness' of an object, *e.g.* it maps any right-hand glove onto a right-hand one and any left-hand glove onto a left-hand one.
(3) A *rotation* is an isometry that 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. In particular, a rotation is called an *N-fold rotation* if the rotation angle is $\varphi = k \times 360^\circ/N$, where k and N are relatively prime integers. A rotation preserves the 'handedness' of any object.
(4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is now called

[1] A real single crystal is still different from a macroscopic crystal. There are dislocations, point defects like vacancies, interstitial atoms or replacements of atoms, and the atoms are never at rest but vibrate. Therefore, the macroscopic crystal is a more-or-less strongly idealized model of the real crystal.

the *screw axis*. The translation vector is called the *screw vector*. A screw rotation has no fixed points. The screw axis is invariant as a whole under the screw rotation but not pointwise.

(5) An N-fold *rotoinversion* is an N-fold rotation coupled with 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*. A rotoinversion changes the handedness by its inversion component: it maps any right-hand glove onto a left-hand one and *vice versa*. Performed twice it results in a rotation. Special rotoinversions are those for $N = 1$ and $N = 2$, which are dealt with separately.

(6) The *inversion* can be considered as a onefold rotoinversion ($N = 1$). The fixed point is called the *inversion centre* or the *centre of symmetry*.

(7) A twofold rotoinversion ($N = 2$) is called a *reflection* or a *reflection through a plane*. It is an isometry which leaves a plane perpendicular to the twofold rotoinversion axis fixed pointwise. This plane is called the *reflection plane* or *mirror plane* and it intersects the rotation axis in the centre of the rotoinversion. Its orientation is described by the direction of its normal vector, *i.e.* of the rotation axis. For a twofold rotoinversion, neither the rotation nor the inversion are symmetry operations themselves. As for any other rotoinversion, the reflection changes the handedness of an 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*. A glide reflection changes the handedness and has no fixed point. The former reflection plane is now called the *glide plane*. Under a glide reflection, the glide plane is invariant as a whole but not pointwise.

Symmetry operations of crystal patterns may belong to any of these isometries. The set of all symmetry operations of a crystal pattern has the following properties: performing two (and thus more) symmetry operations one after the other results in another symmetry operation. Moreover, there is the identity operation in this set, *i.e.* an operation that leaves every point of the space and thus of the crystal pattern fixed. Finally, for any symmetry operation of an object there is an 'inverse' symmetry operation by which its effect is reversed. These properties are necessary for the application of group theory, *cf.* Section 1.2.3.

1.2.2.2. Coordinate systems and coordinates

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. For the plane (two-dimensional space) an origin and two linearly independent (*i.e.* not parallel) basis vectors $\mathbf{a}$, $\mathbf{b}$ (or $\mathbf{a}_1$, $\mathbf{a}_2$) are chosen. Referred to this coordinate system, each point P can be described by three (or two for the plane) coordinates x, y, z (or x_1, x_2, x_3). An object, for example a crystal, can now be described by a continuous or discontinuous function of the coordinates such as the electron density or the coordinates of the centres of the atoms. A mapping can be regarded as an instruction of how to calculate the coordinates $\tilde{x}$, $\tilde{y}$, $\tilde{z}$ of the image point $\tilde{X}$ from the coordinates x, y, z of the original point X.

In contrast to the practice in physics and chemistry, a non-Cartesian coordinate system is usually chosen in crystallography. The primary aim of the choice of the crystallographic coordinate system is to describe the crystal pattern and its set of all symmetry operations in a simple way. This aim holds in particular for the infinitely many symmetry translations of the crystal pattern, which form its *translation group*. Secondary to this aim are equality of the lengths of, and right angles between, the basis vectors.

The vector $\mathbf{t}$ belonging to the translation t is called a *translation vector* or a *lattice vector*. The set of all translation vectors of the crystal pattern is called its *vector lattice* $\mathbf{L}$. Both the translation group and the vector lattice are useful tools for describing the periodicity of the crystals.

For the description of a vector lattice several kinds of bases are in use. Orthonormal bases are not the most convenient, because the coefficients of the lattice vectors may then be any real number. The coefficients of the lattice vectors are more transparent if the basis vectors themselves are lattice vectors.

Definition 1.2.2.2.1. A basis which consists of lattice vectors of a crystal pattern is called a *lattice basis* or a *crystallographic basis*. □

Referred to a lattice basis, each lattice vector $\boldsymbol{t} \in \mathbf{L}$ is a linear combination of the basis vectors with *rational coefficients*. One can even select special bases such that the coefficients of all lattice vectors are integers.

Definition 1.2.2.2.2. A crystallographic basis is called a *primitive basis* if *every* lattice vector has integer coefficients. □

A fundamental feature of vector lattices is that for any lattice in a dimension greater than one an infinite number of primitive bases exists. With certain rules, the choice of a primitive basis can be made unique (reduced bases). In practice, however, the *conventional bases* are not always primitive; the choice of a conventional basis is determined by the matrix parts of the symmetry operations, *cf.* Section 1.2.5.1.

1.2.2.3. The description of mappings

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

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

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

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

This matrix equation is usually abbreviated by

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\,\boldsymbol{x} + \boldsymbol{w}, \tag{1.2.2.3}$$

where

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

Definition 1.2.2.3.1. The matrix $\boldsymbol{W}$ is called the *linear part* or *matrix part*, the column $\boldsymbol{w}$ is the *translation part* or *column part* of a mapping. □

In equations (1.2.2.1) and (1.2.2.3), the coordinates are mixed with the quantities describing the mapping, designated by the letters W_{ik} and w_j or $\boldsymbol{W}$ and $\boldsymbol{w}$. Therefore, one prefers to write equation (1.2.2.3) in the form

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

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 the *Seitz symbol*.

The formulae for the combination of affine mappings and for the inverse of an affine mapping (regular matrix $\boldsymbol{W}$) are obtained by

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1, \quad \tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_3\boldsymbol{x} + \boldsymbol{w}_3$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1) + \boldsymbol{w}_2 = \boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2.$$

From $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, it follows that $\boldsymbol{W}^{-1}\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{W}^{-1}\boldsymbol{w}$ or $\boldsymbol{x} = \boldsymbol{W}^{-1}\tilde{\boldsymbol{x}} - \boldsymbol{W}^{-1}\boldsymbol{w}$.

Using matrix–column pairs, this reads

$$(\boldsymbol{W}_3,\ \boldsymbol{w}_3) = (\boldsymbol{W}_2,\ \boldsymbol{w}_2)(\boldsymbol{W}_1,\ \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1,\ \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2) \qquad (1.2.2.5)$$

and

$$\boldsymbol{x} = (\boldsymbol{W},\ \boldsymbol{w})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{W}',\ \boldsymbol{w}')\tilde{x}$$

or

$$(\boldsymbol{W}',\ \boldsymbol{w}') = (\boldsymbol{W},\ \boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}). \qquad (1.2.2.6)$$

One finds from equations (1.2.2.5) and (1.2.2.6) that the linear parts of the matrix–column pairs transform as one would expect:

(1) the linear part of the product of two matrix–column pairs is the product of the linear parts, *i.e.* if $(\boldsymbol{W}_3,\ \boldsymbol{w}_3) = (\boldsymbol{W}_2,\ \boldsymbol{w}_2)(\boldsymbol{W}_1,\ \boldsymbol{w}_1)$ then $\boldsymbol{W}_3 = \boldsymbol{W}_2\,\boldsymbol{W}_1$;
(2) the linear part of the inverse of a matrix–column pair is the inverse of the linear part, *i.e.* if $(\boldsymbol{X},\ \boldsymbol{x}) = (\boldsymbol{W},\ \boldsymbol{w})^{-1}$, then $\boldsymbol{X} = \boldsymbol{W}^{-1}$. [This relation is included in the first one: from $(\boldsymbol{W},\ \boldsymbol{w})(\boldsymbol{X},\ \boldsymbol{x}) = (\boldsymbol{W}\boldsymbol{X},\ \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}) = (\boldsymbol{I},\ \boldsymbol{o})$ follows $\boldsymbol{X} = \boldsymbol{W}^{-1}$. Here $\boldsymbol{I}$ is the unit matrix and $\boldsymbol{o}$ is the column consisting of zeroes].

These relations will be used in Section 1.2.5.4.

For the column parts, equations (1.2.2.5) and (1.2.2.6) are less convenient:

$$(1)\ \boldsymbol{w}_3 = \boldsymbol{W}_2\,\boldsymbol{w}_1 + \boldsymbol{w}_2; \qquad (2)\ \boldsymbol{w}' = -\boldsymbol{W}^{-1}\boldsymbol{w}.$$

Because of the inconvenience of these relations, it is often preferable to use 'augmented' matrices, by which one can describe the combination of affine mappings and the inverse mapping by the equations of the usual matrix multiplication. These matrices are introduced in the next section.

1.2.2.4. Matrix–column pairs and (n + 1) × (n + 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 are designated by open-face letters in this volume:

$$\mathbb{W} = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \quad \tilde{\mathbb{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{pmatrix}, \quad \mathbb{x} = \begin{pmatrix} x \\ y \\ z \\ \hline 1 \end{pmatrix}. \qquad (1.2.2.7)$$

In order to write equation (1.2.2.3) as $\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}$ with the augmented matrices $\mathbb{W}$, the columns $\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}$ also have to be extended to the augmented columns $\mathbb{x}$ and $\tilde{\mathbb{x}}$. Equations (1.2.2.5) and (1.2.2.6) then become

$$\mathbb{W}_3 = \mathbb{W}_2\,\mathbb{W}_1 \text{ and } (\mathbb{W})^{-1} = (\mathbb{W}^{-1}). \qquad (1.2.2.8)$$

The vertical and horizontal lines in the matrix have no mathematical meaning. They are simply a convenience for separating the matrix part from the column part and from the row '0 0 0 1', and could be omitted.

Augmented matrices are very useful when writing down general formulae which then become more transparent and more elegant. However, the matrix–column pair formalism is, in general, advantageous for practical calculations.

For the augmented columns of vector coefficients, see Section 1.2.2.6.

1.2.2.5. Isometries

Isometries are special affine mappings, as in Definition 1.2.2.1.1. The matrix $\boldsymbol{W}$ of an isometry has to fulfil conditions which depend on the coordinate basis. These conditions are:

(1) A basis $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ is characterized by the scalar products $(\mathbf{a}_j\,\mathbf{a}_k)$ of its basis vectors or by its *lattice parameters* a, b, c, α, β and γ. Here a, b, c are the lengths of the basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and α, β and γ are the angles between $\mathbf{a}_2$ and $\mathbf{a}_3$, $\mathbf{a}_3$ and $\mathbf{a}_1$, $\mathbf{a}_1$ and $\mathbf{a}_2$, respectively. The *metric matrix* $\boldsymbol{M}$ [called $\mathbf{G}$ in *International Tables for Crystallography* Volume A (2005) (abbreviated as *IT* A), Chapter 9.1] is the (3 × 3) matrix which consists of the scalar products of the basis vectors:

$$\boldsymbol{M} = \begin{pmatrix} a^2 & a\,b\,\cos\gamma & a\,c\,\cos\beta \\ b\,a\,\cos\gamma & b^2 & b\,c\,\cos\alpha \\ c\,a\,\cos\beta & c\,b\,\cos\alpha & c^2 \end{pmatrix}.$$

If $\boldsymbol{W}$ is the matrix part of an isometry, referred to the basis $(\mathbf{a}_1,\ \mathbf{a}_2,\ \mathbf{a}_3)$, then $\boldsymbol{W}$ must fulfil the condition $\boldsymbol{W}^{\mathrm{T}}\boldsymbol{M}\,\boldsymbol{W} = \boldsymbol{M}$, where $\boldsymbol{W}^{\mathrm{T}}$ is the transpose of $\boldsymbol{W}$.
(2) For the *determinant* of $\boldsymbol{W}$, $\det(\boldsymbol{W}) = \pm 1$ must hold; $\det(\boldsymbol{W}) = +1$ for the identity, translations, rotations and screw rotations; $\det(\boldsymbol{W}) = -1$ for inversions, reflections, glide reflections and rotoinversions.
(3) For the *trace*, $\mathrm{tr}(\boldsymbol{W}) = W_{11} + W_{22} + W_{33} = \pm(1 + 2\cos\varphi)$ holds, where φ is the rotation angle; the + sign applies if $\det(\boldsymbol{W}) = +1$ and the − sign if $\det(\boldsymbol{W}) = -1$.

Algorithms for the determination of the kind of isometry from a given matrix–column pair and for the determination of the matrix–column pair for a given isometry can be found in *IT* A, Part 11 or in Hahn & Wondratschek (1994).

1.2.2.6. Vectors and vector coefficients

In crystallography, vectors and their coefficients as well as points and their coordinates are used for the description of crystal structures. Vectors represent translation shifts, distance and Patterson vectors, reciprocal-lattice vectors *etc.* With respect to a given basis a vector has three coefficients. In contrast to the coordinates of a point, these coefficients do not change if the origin of the coordinate system is shifted. 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: the vector from the point P to the point Q has the coefficients $v_1 = q_1 - p_1,\ v_2 = q_2 - p_2,\ v_3 = q_3 - p_3,\ 1 - 1$. Thus, the column of the coefficients of a vector is not augmented by '1' but by '0'. Therefore, 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 $\mathbf{v} = \overrightarrow{P\,Q}$ is mapped onto the vector $\tilde{\mathbf{v}} = \overrightarrow{\tilde{P}\,\tilde{Q}}$ by transforming its coefficients by $\tilde{\boldsymbol{v}} = \boldsymbol{W}\boldsymbol{v}$, because the coefficients w_j are multiplied by the number '0' augmenting the column $\boldsymbol{v} = (v_j)$. Indeed, the distance vector $\mathbf{v} = \overrightarrow{P\,Q}$ 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 5.1 and 5.2, and in Hahn & Wondratschek (1994).

Let a coordinate system be given with a basis $(\mathbf{a}_1,\ \mathbf{a}_2,\ \mathbf{a}_3)^{\mathrm{T}}$ and an origin O.[2] 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 $(\mathbf{a}'_1,\ \mathbf{a}'_2,\ \mathbf{a}'_3)^{\mathrm{T}}$ 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 $\boldsymbol{p} = \overrightarrow{O\,O'}$ be the column of coefficients for the vector from the old origin O to the new origin O' and let

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

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

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

Then the following equations hold:

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

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

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

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

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

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

These equations read in the augmented-matrix formalism

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

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. A group is a set of elements with a *law of composition*, by which to any two elements a third element is uniquely assigned. 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* (Ledermann, 1976; Ledermann & Weir, 1996) is recommended. The book *Symmetry of Crystals. Introduction to International Tables for Crystallography, Vol. A* by Hahn & Wondratschek (1994)

[2] 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 $(h,\ k,\ l)^{\mathrm{T}}$ or $(\mathbf{a},\ \mathbf{b},\ \mathbf{c})^{\mathrm{T}}$, even if they are written in a row.