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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*

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

(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 $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}}$ 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 $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\mathrm{T}}$ 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 $\boldsymbol{p} = \overrightarrow{OO'}$ 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 $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\mathrm{T}}$ to the old basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}}$ according to

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

[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 $(h, k, l)^{\mathrm{T}}$ or $(\mathbf{a}, \mathbf{b}, \mathbf{c})^{\mathrm{T}}$, 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.

(2) The *associative law* is always fulfilled for the composition of geometric mappings. If $g_j,\ g_k,\ g_m \in \mathcal{G}$, then $(g_j\,g_k)\,g_m = g_j\,(g_k\,g_m) = g_q$ for any triplet j, k, m. Therefore, the parentheses are not necessary, one can write $g_j\,g_k\,g_m = g_q$. In general, however, the sequence of the symmetry operations must not be changed. Thus, in general $g_j\,g_k\,g_m \neq g_j\,g_m\,g_k$.

(3) The *unit element* or *neutral element* $e \in \mathcal{G}$ is the identity operation which maps each point onto itself, *i.e.* leaves each point invariant.

(4) The isometry which reverses a given symmetry operation $g \in \mathcal{G}$ is also a symmetry operation of $\mathcal{G}$ and is called the *inverse* symmetry operation g^{-1} of g. It has the property $g\,g^{-1} = g^{-1}\,g = e$.

The number of elements of a group $\mathcal{G}$ is called its *order* $|\mathcal{G}|$. The order of a group may be finite, *e.g.* 24 for the symmetry operations of a regular tetrahedron, or infinite, *e.g.* for any space group because of its infinite set of translations. If the relation $g_k\,g_j = g_j\,g_k$ is fulfilled for all pairs of elements of a group $\mathcal{G}$, then $\mathcal{G}$ is called a *commutative* or an *Abelian* group.

For groups of higher order, it is usually inappropriate and for groups of infinite order it is impossible to list all elements of a group. The following definition nearly always reduces the set of group elements to be listed explicitly to a small set.

Definition 1.2.3.1.1. A set $\mathcal{S} = \{g_p,\ g_q,\ \ldots\} \in \mathcal{G}$ such that every element of $\mathcal{G}$ can be obtained by composition of the elements of $\mathcal{S}$ and their inverses is called a *set of generators* of $\mathcal{G}$. The elements $g_i \in \mathcal{S}$ are called *generators* of $\mathcal{G}$. □

A group is *cyclic* if it consists of the unit element e and all powers of one element g:

$$\mathcal{C}(g) = \{\ \ldots\ g^{-3},\ g^{-2},\ g^{-1},\ e,\ g^1,\ g^2,\ g^3,\ \ldots\ \}.$$

If there is an integer number $n > 0$ with $g^n = e$ and n is the smallest number with this property, then the group $\mathcal{C}(g)$ has the *finite order n*. Let g^{-k} with $0 < k < n$ be the inverse element of g^k where n is the order of g. Because $g^{-k} = g^n\,g^{-k} = g^{n-k} = g^m$ with $n = m + k$, the elements of a cyclic group of finite order can all be written as positive powers of the generator g. Otherwise, if such an integer n does not exist, the group $\mathcal{C}(g)$ is of *infinite order* and the positive powers g^k are different from the negative ones g^{-m}.

In the same way, from any element $g_j \in \mathcal{G}$ its cyclic group $\mathcal{C}(g_j)$ can be generated even if $\mathcal{G}$ is not cyclic itself. The order of this group $\mathcal{C}(g_j)$ is called the *order of the element* g_j.

1.2.3.2. *Group isomorphism and homomorphism*

A finite group $\mathcal{G}$ of small order may be conveniently visualized by its *multiplication table*, *group table* or *Cayley table*. An example is shown in Table 1.2.3.1.

The multiplication tables can be used to define one of the most important relations between two groups, the isomorphism of groups. This can be done by comparing the multiplication tables of the two groups.

Definition 1.2.3.2.1. Two groups are *isomorphic* if one can arrange the rows and columns of their multiplication tables such that these tables are equal, apart from the names or symbols of the group elements. □

Multiplication tables are useful only for groups of small order. To define 'isomorphism' for arbitrary groups, one can formulate the relations expressed by the multiplication tables in a more abstract way.

Table 1.2.3.1. *Multiplication table of a group*

The group elements $g \in \mathcal{G}$ are listed at the top of the table and in the same sequence on the left-hand side; the unit element 'e' is listed first. The table is thus a square array. The product $g_k\,g_j$ of any pair of elements is listed at the intersection of the kth row and the jth column.
It can be shown that each group element is listed exactly once in each row and once in each column of the table. In the row of an element $g \in \mathcal{G}$, the unit element e appears in the column of g^{-1}. If $(g)^2 = e$, *i.e.* $g = g^{-1}$, e appears on the main diagonal. The multiplication table of an Abelian group is symmetric about the main diagonal.

$\mathcal{G}$	e	a	b	c	$\ldots$
e	e	a	b	c	$\ldots$
a	a	a^2	ab	ac	$\ldots$
b	b	ba	b^2	bc	$\ldots$
c	c	ca	cb	c^2	$\ldots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

The 'same multiplication table' for the groups $\mathcal{G}$ and $\mathcal{G}'$ means that there is a reversible mapping $g_q \longleftrightarrow g'_q$ of the elements $g_q \in \mathcal{G}$ and $g'_q \in \mathcal{G}'$ such that $(g_j\,g_k)' = g'_j\,g'_k$ holds for any pair of indices j and k. In words:

Definition 1.2.3.2.2. Two groups $\mathcal{G}$ and $\mathcal{G}'$ are isomorphic if there is a reversible mapping of $\mathcal{G}$ onto $\mathcal{G}'$ such that for any pair of elements of $\mathcal{G}$ the image of the product is equal to the product of the images. □

Isomorphic groups have the same order. By isomorphism the set of all groups is classified into *isomorphism types* or *isomorphism classes* of groups. Such a class is often called an *abstract group*.

The isomorphism between the space groups and the corresponding matrix groups makes an analytical treatment of crystallographic symmetry possible. Moreover, the isomorphism of different space groups allows one to classify the infinite number of space groups into a finite number of *isomorphism types of space groups*, which is one of the bases of crystallography, see Section 1.2.5.

Isomorphism provides a very strong relation between groups: the groups are identical in their group-theoretical properties. One can weaken this relation by omitting the condition of reversibility of the mapping. One then admits that more than one element of the group $\mathcal{G}$ is mapped onto the same element of $\mathcal{G}'$. This concept leads to the definition of homomorphism.

Definition 1.2.3.2.3. A mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$ is called *homomorphic*, and $\mathcal{G}'$ is called a *homomorphic image* of the group $\mathcal{G}$, if for any pair of elements of $\mathcal{G}$ the image of the product is equal to the product of the images and if any element of $\mathcal{G}'$ is the image of at least one element of $\mathcal{G}$. The relation of $\mathcal{G}$ and $\mathcal{G}'$ is called a *homomorphism*. More formally: For the mapping $\mathcal{G}$ onto $\mathcal{G}'$, $(g_j\,g_k)' = g'_j\,g'_k$ holds. □

The formulation 'mapping onto' implies that each element $g' \in \mathcal{G}'$ occurs among the images of the elements $g \in \mathcal{G}$ at least once.[2]

The very important concept of homomorphism is discussed further in Lemma 1.2.4.4.3. The crystallographic point groups are homomorphic images of the space groups, see Section 1.2.5.4.

[2] In mathematics, the term 'homomorphism' includes mappings of a group $\mathcal{G}$ *into* a group $\mathcal{G}'$, *i.e.* mappings in which not every $g' \in \mathcal{G}'$ is the image of some element of $g \in \mathcal{G}$. The term 'homomorphism onto' defined above is also known as an *epimorphism*, *e.g.* in Ledermann (1976). In the older literature the term 'multiple isomorphism' can also be found.

references