

1. SPACE GROUPS AND THEIR SUBGROUPS

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 $\tilde{\mathbf{x}} \equiv \mathbf{W}\mathbf{x} + \mathbf{w}$ according to equation (1.2.2.3), then the vector $\mathbf{v} = \overrightarrow{PQ}$ is mapped onto the vector $\tilde{\mathbf{v}} = \overrightarrow{\tilde{P}\tilde{Q}}$ by transforming its coefficients by $\tilde{\mathbf{v}} = \mathbf{W}\mathbf{v}$, because the coefficients w_j are multiplied by the number '0' augmenting the column $\mathbf{v} = (v_j)$. Indeed, the 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 \mathbf{x} and the vector coefficients \mathbf{v} is not visible in the equations where the symbols \mathbf{x} and \mathbf{v} are used, but is obvious only if the columns are written in full, *viz*

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

- (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 $\tilde{\mathbf{v}} = \mathbf{W}\mathbf{v}$ is called an *orthogonal mapping* if \mathbf{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 $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^T$ and an origin O .² Referred to this coordinate system, the column of coordinates of a point P is \mathbf{x} ; the matrix and column parts describing a symmetry operation are \mathbf{W} and \mathbf{w} according to

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

equations (1.2.2.1) to (1.2.2.3), and the column of vector coefficients is \mathbf{v} , see Section 1.2.2.6. A new coordinate system may be introduced with the basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^T$ and the origin O' . Referred to the new coordinate system, the column of coordinates of the point P is \mathbf{x}' , the symmetry operation is described by \mathbf{W}' and \mathbf{w}' and the column of vector coefficients is \mathbf{v}' .

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

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

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

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

Then the following equations hold:

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

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

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

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

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

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

These equations read in the augmented-matrix formalism

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

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 (\mathbf{I}, \mathbf{v}) , *i.e.* $\mathbf{W} = \mathbf{I}$, $\mathbf{w} = \mathbf{v}$. 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, (\mathbf{I}, \mathbf{p}) , because $(\mathbf{I}, \mathbf{v})' = (\mathbf{I}, \mathbf{v})$ holds. Moreover, under a general coordinate transformation the origin shift is not effective: in equation (1.2.2.13) only $\mathbf{v}' = \mathbf{P}^{-1}\mathbf{v}$ remains because of the equality $\mathbf{W} = \mathbf{I}$.

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)

1.2. GENERAL INTRODUCTION TO THE SUBGROUPS OF SPACE GROUPS

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 k th row and the j th 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	...
e	e	a	b	c	...
a	a	a^2	ab	ac	...
b	b	ba	b^2	bc	...
c	c	ca	cb	c^2	...
\vdots	\vdots	\vdots	\vdots	\vdots	\ddots

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 italic 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, for example 24 for the symmetry operations of a regular tetrahedron, or infinite, for example 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 $\mathcal{S} = \{g_p, g_q, \dots\} \in \mathcal{G}$ 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} . \square

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

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

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. \square

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.

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. \square

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

1. SPACE GROUPS AND THEIR SUBGROUPS

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. \square

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.³

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.

1.2.4. Subgroups

1.2.4.1. Definition

There may be sets of elements $g_k \in \mathcal{G}$ that do not constitute the full group \mathcal{G} but nevertheless fulfil the group postulates for themselves.

Definition 1.2.4.1.1. A subset \mathcal{H} of elements of a group \mathcal{G} is called a *subgroup* \mathcal{H} of \mathcal{G} if it fulfils the group postulates with respect to the law of composition of \mathcal{G} . \square

Remarks

- (1) The group \mathcal{G} is considered to be one of its own subgroups. If subgroups \mathcal{H}_j are discussed where \mathcal{G} is included among the subgroups, we write $\mathcal{H}_j \leq \mathcal{G}$ or $\mathcal{G} \geq \mathcal{H}_j$. If \mathcal{G} is excluded from the set $\{\mathcal{H}_j\}$ of its subgroups, we write $\mathcal{H}_j < \mathcal{G}$ or $\mathcal{G} > \mathcal{H}_j$. A subgroup $\mathcal{H}_j < \mathcal{G}$ is called a *proper subgroup* of \mathcal{G} .
- (2) In a relation $\mathcal{G} \geq \mathcal{H}$ or $\mathcal{G} > \mathcal{H}$, \mathcal{G} is called a *supergroup* of \mathcal{H} . The symbols \leq , \geq , $<$ and $>$ are used for supergroups in the same way as they are used for subgroups, cf. Section 2.1.6.
- (3) A subgroup of a finite group is finite. A subgroup of an infinite group may be finite or infinite.
- (4) A subset \mathcal{K} of elements $g_k \in \mathcal{G}$ which does not necessarily form a group is designated by the symbol $\mathcal{K} \subset \mathcal{G}$.

Definition 1.2.4.1.2. A subgroup $\mathcal{H} < \mathcal{G}$ is a *maximal subgroup* if no group \mathcal{Z} exists for which $\mathcal{H} < \mathcal{Z} < \mathcal{G}$ holds. If \mathcal{H} is a maximal subgroup of \mathcal{G} , then \mathcal{G} is a *minimal supergroup* of \mathcal{H} . \square

This definition is very important for the tables of this volume, as only maximal subgroups of space groups are listed. If all maximal subgroups are known for any given space group, then any general subgroup $\mathcal{H} < \mathcal{G}$ can be obtained by a (finite) chain of maximal subgroups between \mathcal{G} and \mathcal{H} , see Section

³ 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) and Ledermann & Weir (1996). In the older literature the term ‘multiple isomorphism’ can also be found.

1.2.6.2. Moreover, the relations between a space group and its maximal subgroups are particularly transparent, cf. Lemma 1.2.8.1.3.

1.2.4.2. Coset decomposition and normal subgroups

Let $\mathcal{H} < \mathcal{G}$ be a subgroup of \mathcal{G} of order $|\mathcal{H}|$. Because \mathcal{H} is a proper subgroup of \mathcal{G} there must be elements $g_q \in \mathcal{G}$ that are not elements of \mathcal{H} . Let $g_2 \in \mathcal{G}$ be one of them. Then the set of elements $g_2 \mathcal{H} = \{g_2 h_j \mid h_j \in \mathcal{H}\}$ ⁴ is a subset of elements of \mathcal{G} with the property that all its elements are different and that the sets \mathcal{H} and $g_2 \mathcal{H}$ have no element in common. Thus, the set $g_2 \mathcal{H}$ also contains $|\mathcal{H}|$ elements of \mathcal{G} . If there is another element $g_3 \in \mathcal{G}$ which belongs neither to \mathcal{H} nor to $g_2 \mathcal{H}$, one can form another set $g_3 \mathcal{H} = \{g_3 h_j \mid h_j \in \mathcal{H}\}$. All elements of $g_3 \mathcal{H}$ are different and none occurs already in \mathcal{H} or in $g_2 \mathcal{H}$. This procedure can be continued until each element $g_r \in \mathcal{G}$ belongs to one of these sets. In this way the group \mathcal{G} can be partitioned, such that each element $g \in \mathcal{G}$ belongs to exactly one of these sets.

Definition 1.2.4.2.1. The partition just described is called a *decomposition* ($\mathcal{G} : \mathcal{H}$) into *left cosets* of the group \mathcal{G} relative to the group \mathcal{H} . The sets $g_p \mathcal{H}$, $p = 1, \dots, i$ are called *left cosets*, because the elements $h_j \in \mathcal{H}$ are multiplied with the new elements from the left-hand side. The procedure is called a *decomposition into right cosets* $\mathcal{H} g_s$ if the elements $h_j \in \mathcal{H}$ are multiplied with the new elements g_s from the right-hand side. The elements g_p or g_s are called the *coset representatives*. The number of cosets is called the *index* $i = |\mathcal{G} : \mathcal{H}|$ of \mathcal{H} in \mathcal{G} . \square

Remarks

- (1) The group $\mathcal{H} = g_1 \mathcal{H}$ with $g_1 = e$ is the first coset for both kinds of decomposition. It is the only coset which forms a group by itself.
- (2) All cosets have the same *length*, i.e. the same number of elements, which is equal to $|\mathcal{H}|$, the order of \mathcal{H} .
- (3) The index i is the same for both right and left decompositions. In *ITA* and in this volume, the index is frequently designated by the symbol $[i]$.
- (4) A coset does not depend on its representative element; starting from any of its elements will result in the same coset. The right cosets may be different from the left ones and the representatives of the right and left cosets may also differ.
- (5) If the order $|\mathcal{G}|$ of \mathcal{G} is infinite, then either the order $|\mathcal{H}|$ of \mathcal{H} or the index $i = |\mathcal{G} : \mathcal{H}|$ of \mathcal{H} in \mathcal{G} or both are infinite.
- (6) The coset decomposition of a space group \mathcal{G} relative to its translation subgroup $\mathcal{T}(\mathcal{G})$ is fundamental in crystallography, cf. Section 1.2.5.4.

From its definition and from the properties of the coset decomposition mentioned above, one immediately obtains the fundamental theorem of Lagrange (for another formulation, see Chapter 1.4):

Lemma 1.2.4.2.2. Lagrange’s theorem: Let \mathcal{G} be a group of finite order $|\mathcal{G}|$ and $\mathcal{H} < \mathcal{G}$ a subgroup of \mathcal{G} of order $|\mathcal{H}|$. Then $|\mathcal{H}|$ is a divisor of $|\mathcal{G}|$ and the equation $|\mathcal{H}| \times i = |\mathcal{G}|$ holds where $i = |\mathcal{G} : \mathcal{H}|$ is the index of \mathcal{H} in \mathcal{G} . \square

A special situation exists when the left and right coset decompositions of \mathcal{G} relative to \mathcal{H} result in the partition of \mathcal{G} into the same cosets:

⁴ The formulation $g_2 \mathcal{H} = \{g_2 h_j \mid h_j \in \mathcal{H}\}$ means: ‘ $g_2 \mathcal{H}$ is the set of the products $g_2 h_j$ of g_2 with all elements $h_j \in \mathcal{H}$.’