International Tables for Crystallography (2006). Vol. A, Chapter 8.1, pp. 720–725.

8.1. Basic concepts

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8.1.1. Introduction

The aim of this part is to define and explain some of the concepts and terms frequently used in crystallography, and to present some basic knowledge in order to enable the reader to make best use of the space-group tables.

The reader will be assumed to have some familiarity with analytical geometry and linear algebra, including vector and matrix calculus. Even though one can solve a good number of practical crystallographic problems without this knowledge, some mathematical insight is necessary for a more thorough understanding of crystallography. In particular, the application of symmetry theory to problems in crystal chemistry and crystal physics requires a background of group theory and, sometimes, also of representation theory.

The symmetry of crystals is treated in textbooks by different methods and at different levels of complexity. In this part, a mainly algebraic approach is used, but the geometric viewpoint is presented also. The algebraic approach has two advantages: it facilitates computer applications and it permits statements to be formulated in such a way that they are independent of the dimension of the space. This is frequently done in this part.

A great selection of textbooks and monographs is available for the study of crystallography. Only Giacovazzo (2002) and Vainshtein (1994) will be mentioned here.

Surveys of the history of crystallographic symmetry can be found in Burckhardt (1988) and Lima-de-Faria (1990).

In addition to books, many programs exist by which crystallographic computations can be performed. For example, the programs can be used to derive the classes of point groups, space groups, lattices (Bravais lattices) and crystal families; to calculate the subgroups of point groups and space groups, Wyckoff positions, irreducible representations *etc.* The mathematical program packages *GAP* (Groups, Algorithms and Programming), in particular *CrystGap*, and *Carat* (Crystallographic Algorithms and Tables) are examples of powerful tools for the solution of problems of crystallographic symmetry. For *GAP*, see http://www.gap-system.org/; for *Carat*, see http://wwwb.math.rwth-aachen.de/carat/. Other programs are provided by the crystallographic server in Bilbao: http://www.cryst.ehu.es/cryst/.

Essential for the determination of crystal structures are extremely efficient program systems that implicitly make use of crystallographic (and noncrystallographic) symmetries.

In this part, as well as in the space-group tables of this volume, 'classical' crystallographic groups in three, two and one dimensions are described, *i.e.* space groups, plane groups, line groups and their associated point groups. In addition to three-dimensional crystallography, which is the basis for the treatment of crystal structures, crystallography of two- and one-dimensional space is of practical importance. It is encountered in sections and projections of crystal structures, in mosaics and in frieze ornaments.

There are several expansions of 'classical' crystallographic groups (groups of motions) that are not treated in this volume but will or may be included in future volumes of the *IT* series.

(*a*) Generalization of crystallographic groups to spaces of dimension $n > 3$ is the field of n-dimensional crystallography. Some results are available. The crystallographic symmetry operations for spaces of any dimension n have already been derived by Hermann (1949). The crystallographic groups of four-dimensional space are also completely known and have been tabulated by Brown *et al.* (1978) and Schwarzenberger (1980). The present state of the art and results for higher dimensions are described by Opgenorth *et al.* (1998), Plesken & Schulz (2000) and Souvignier (2003). Some of their results are displayed in Table 8.1.1.1.

(*b*) One can deal with groups of motions whose lattices of translations have lower dimension than the spaces on which the groups act. This expansion yields the *subperiodic groups*. In particular, there are frieze groups (groups in a plane with one-dimensional translations), rod groups (groups in space with one-dimensional translations) and layer groups (groups in space with two-dimensional translations). These subperiodic groups are treated in *IT* E (2002) in a similar way to that in which line groups, plane groups and space groups are treated in this volume. Subperiodic groups are strongly related to 'groups of generalized symmetry'.

(*c*) Incommensurate phases, *e.g.* modulated structures or inclusion compounds, as well as quasicrystals, have led to an extension of crystallography beyond periodicity. Such structures are not really periodic in three-dimensional space but their symmetry may be described as that of an n-dimensional periodic structure, *i.e.* by an n-dimensional space group. In practical cases, $n = 4$, 5 or 6 holds. The crystal structure is then an irrational three-dimensional section through the n-dimensional periodic structure. The description by crystallographic groups of higher-dimensional spaces is thus of practical interest, *cf.* Janssen *et al.* (2004), van Smaalen (1995) or Yamamoto (1996).

(*d*) Generalized symmetry. Other generalizations of crystallographic symmetry combine the geometric symmetry operations with changes of properties: black–white groups, colour groups *etc.* They are treated in the classical book by Shubnikov & Koptsik (1974). Janner (2001) has given an overview of further generalizations.

8.1.2. Spaces and motions

Crystals are objects in the physical three-dimensional space in which we live. A model for the mathematical treatment of this space is the so-called *point space*, which in crystallography is known as *direct* or *crystal space*. In this space, the structures of finite real crystals are idealized as infinite perfect three-dimensional crystal structures (*cf.* Section 8.1.4). This implies that for crystal structures and their symmetries the surfaces of crystals as well as their defects and imperfections are neglected; for most applications, this is an excellent approximation.

The description of crystal structures and their symmetries is not as simple as it appears at first sight. It is useful to consider not only

Table 8.1.1.1. *Number of crystallographic classes for dimensions 1 to 6*

The numbers are those of the *affine* equivalence classes. The numbers for the enantiomorphic pairs are given in parentheses preceded by a + sign (Souvignier, 2003).

Dimension of space	Crystal families	Lattice (Bravais) types	(Geometric) crystal classes	Arithmetic crystal classes	Space-group types
1	1	1	2	2	2
2	4	5	10	13	17
3	6	14	32	73	(+11) 219
4	(+6) 23	(+10) 64	(+44) 227	(+70) 710	(+111) 4783
5	32	189	955	6079	222018
6	91	841	7104	(+30) 85311	(+7052) 28927922

the above-mentioned point space but also to introduce simultaneously a *vector space* which is closely connected with the point space. Crystallographers are used to working in both spaces: crystal structures are described in point space, whereas face normals, translation vectors, Patterson vectors and reciprocal-lattice vectors are elements of vector spaces.

In order to carry out crystallographic calculations it is necessary to have a *metrics* in point space. Metrical relations, however, are most easily introduced in vector space by defining scalar products between vectors from which the length of a vector and the angle between two vectors are derived. The connection between the vector space $\mathbf{V}^n$ and the point space E^n transfers both the metrics and the dimension of $\mathbf{V}^n$ onto the point space E^n in such a way that distances and angles in point space may be calculated.

The connection between the two spaces is achieved in the following way:

(i) To any two points P and Q of the point space E^n a vector $\overrightarrow{PQ} = \mathbf{r}$ of the vector space $\mathbf{V}^n$ is attached.

(ii) For each point P of E^n and each vector $\mathbf{r}$ of $\mathbf{V}^n$ there is exactly one point Q of E^n for which $\overrightarrow{PQ} = \mathbf{r}$ holds.

(iii) $\overrightarrow{PQ} + \overrightarrow{QR} = \overrightarrow{PR}$.

The distance between two points P and Q in point space is given by the length $|\overrightarrow{PQ}| = (\overrightarrow{PQ}, \overrightarrow{PQ})^{1/2}$ of the attached vector $\overrightarrow{PQ}$ in vector space. In this expression, $(\overrightarrow{PQ}, \overrightarrow{PQ})$ is the scalar product of $\overrightarrow{PQ}$ with itself.

The angle determined by P, Q and R with vertex Q is obtained from

$$\cos(P,Q,R) = \cos(\overrightarrow{QP}, \overrightarrow{QR}) = \frac{(\overrightarrow{QP}, \overrightarrow{QR})}{|\overrightarrow{QP}| \cdot |\overrightarrow{QR}|}.$$

Here, $(\overrightarrow{QP}, \overrightarrow{QR})$ is the scalar product between $\overrightarrow{QP}$ and $\overrightarrow{QR}$. Such a point space is called an n-dimensional *Euclidean space*.

If we select in the point space E^n an arbitrary point O as the *origin*, then to each point X of E^n a unique vector $\overrightarrow{OX}$ of $\mathbf{V}^n$ is assigned, and there is a one-to-one correspondence between the points X of E^n and the vectors $\overrightarrow{OX}$ of $\mathbf{V}^n : X \leftrightarrow \overrightarrow{OX} = \mathbf{x}$.

Referred to a vector basis $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of $\mathbf{V}^n$, each vector $\mathbf{x}$ is uniquely expressed as $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ or, using matrix multiplication,* $\mathbf{x} = (\mathbf{a}_1, \ldots, \mathbf{a}_n)\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$.

Referred to the coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ of E^n, Fig. 8.1.2.1, each point X is uniquely described by the column of coordinates

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}.$$

Thus, the real numbers x_i are either the *coefficients of the vector* $\mathbf{x}$ of $\mathbf{V}^n$ or the *coordinates of the point* X of E^n.

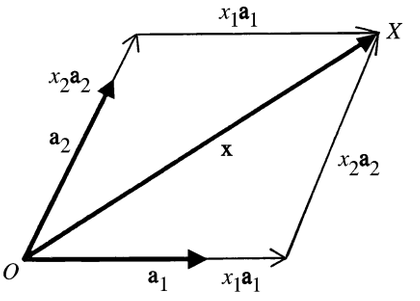

Fig. 8.1.2.1. Representation of the point X with respect to origin O by the vector $\overrightarrow{OX} = \mathbf{x}$. The vector $\mathbf{x}$ is described with respect to the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$ by the coefficients x_1, x_2. The coordinate system $(O, \mathbf{a}_1, \mathbf{a}_2)$ of the point space E^2 consists of the point O of E^2 and the vector basis $\{\mathbf{a}_1, \mathbf{a}_2\}$ of $\mathbf{V}^2$.

An instruction assigning uniquely to each point X of the point space E^n an 'image' point $\tilde{X}$, whereby all distances are left invariant, is called an *isometry*, an *isometric mapping* or a *motion* M of E^n. Motions are invertible, *i.e.*, for a given motion $\mathsf{M} : X \rightarrow \tilde{X}$, the inverse motion $\mathsf{M}^{-1} : \tilde{X} \rightarrow X$ exists and is unique.

Referred to a coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$, any motion $X \rightarrow \tilde{X}$ may be described in the form

$$\begin{array}{lcccccc} \tilde{x}_1 & = & W_{11}x_1 & + \ldots + & W_{1n}x_n & + & w_1 \\ \vdots & = & \vdots & & \vdots & & \vdots \\ \tilde{x}_n & = & W_{n1}x_1 & + \ldots + & W_{nn}x_n & + & w_n. \end{array}$$

In matrix formulation, this is expressed as

$$\begin{pmatrix} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \end{pmatrix} = \begin{pmatrix} W_{11} & \ldots & W_{1n} \\ \vdots & & \vdots \\ W_{n1} & \ldots & W_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} + \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix}$$

or, in abbreviated form, as $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, where $\tilde{\boldsymbol{x}}$, $\boldsymbol{x}$ and $\boldsymbol{w}$ are all $(n \times 1)$ columns and $\boldsymbol{W}$ is an $(n \times n)$ square matrix. One often writes this in even more condensed form as $\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}$, or $\tilde{\boldsymbol{x}} = (\boldsymbol{W}|\boldsymbol{w})\boldsymbol{x}$; here, $(\boldsymbol{W}|\boldsymbol{w})$ is called the *Seitz symbol*.

A motion consists of a *rotation part* or *linear part* and a *translation part*. If the motion is represented by $(\boldsymbol{W}, \boldsymbol{w})$, the matrix $\boldsymbol{W}$ describes the rotation part of the motion and is called the *matrix part* of $(\boldsymbol{W}, \boldsymbol{w})$. The column $\boldsymbol{w}$ describes the translation part of the motion and is called the *vector part* or *column part* of $(\boldsymbol{W}, \boldsymbol{w})$. For a given motion, the matrix $\boldsymbol{W}$ depends only on the choice of the basis vectors, whereas the column $\boldsymbol{w}$ in general depends on the choice of the basis vectors *and* of the origin O; *cf.* Section 8.3.1.

It is possible to combine the $(n \times 1)$ column and the $(n \times n)$ matrix representing a motion into an $(n+1) \times (n+1)$ square matrix which is called the *augmented matrix*. The system of equations $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ may then be expressed in the following form:

$$\left(\begin{array}{c} \tilde{x}_1 \\ \vdots \\ \tilde{x}_n \\ \hline 1 \end{array}\right) = \left(\begin{array}{c|c} & w_1 \\ \boldsymbol{W} & \vdots \\ & w_n \\ \hline 0 \ldots 0 & 1 \end{array}\right) \left(\begin{array}{c} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{array}\right)$$

or, in abbreviated form, by $\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}$. The augmentation is done in two steps. First, the $(n \times 1)$ column $\boldsymbol{w}$ is attached to the $(n \times n)$ matrix and then the matrix is made square by attaching the $[1 \times (n+1)]$ row $(0 \ldots 0\ 1)$. Similarly, the $(n \times 1)$ columns $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$

* For this volume, the following conventions for the writing of vectors and matrices have been adopted:

(i) point coordinates and vector coefficients are written as $(n \times 1)$ column matrices;

(ii) the vectors of the vector basis are written as a $(1 \times n)$ row matrix;

(iii) *all* running indices are written as subscripts.

It should be mentioned that other conventions are also found in the literature, *e.g.* interchange of row and column matrices and simultaneous use of subscripts and superscripts for running indices.

have to be augmented to $[(n+1)\times 1]$ columns $\mathbb{x}$ and $\tilde{\mathbb{x}}$. The motion is now described by the one matrix $\mathbb{W}$ instead of the pair $(\boldsymbol{W}, \boldsymbol{w})$.

If the motion M is described by $\mathbb{W}$, the 'inverse motion' M^{-1} is described by $\mathbb{W}^{-1}$, where $(\boldsymbol{W},\boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1}, -\boldsymbol{W}^{-1}\boldsymbol{w})$. Successive application of two motions, W_1 and W_2, results in another motion W_3:

$$\tilde{X} = \mathsf{W}_1 X \text{ and } \tilde{\tilde{X}} = \mathsf{W}_2\tilde{X} = \mathsf{W}_2\mathsf{W}_1 X = \mathsf{W}_3 X.$$

with $\mathsf{W}_3 = \mathsf{W}_2\mathsf{W}_1$.

This can be described in matrix notation as follows

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1$$

and

$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2 = \boldsymbol{W}_3\boldsymbol{x} + \boldsymbol{w}_3,$$

with $(\boldsymbol{W}_3, \boldsymbol{w}_3) = (\boldsymbol{W}_2\boldsymbol{W}_1, \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2)$ or

$$\tilde{\mathbb{x}} = \mathbb{W}_1\mathbb{x} \text{ and } \tilde{\tilde{\mathbb{x}}} = \mathbb{W}_2\tilde{\mathbb{x}} = \mathbb{W}_2\mathbb{W}_1\mathbb{x} = \mathbb{W}_3\mathbb{x}$$

with $\mathbb{W}_3 = \mathbb{W}_2\mathbb{W}_1$.

It is a special advantage of the augmented matrices that successive application of motions is described by the product of the corresponding augmented matrices.

A point X is called a *fixed point* of the mapping M if it is invariant under the mapping, *i.e.* $\tilde{X} = X$.

In an n-dimensional Euclidean space E^n, three types of motions can be distinguished:

(1) *Translation.* In this case, $\boldsymbol{W} = \boldsymbol{I}$, where $\boldsymbol{I}$ is the unit matrix; the vector $\mathbf{w} = w_1\mathbf{a}_1 + \ldots + w_n\mathbf{a}_n$ is called the *translation vector.*

(2) *Motions with at least one fixed point.* In E^1, E^2 and E^3, such motions are called proper motions or *rotations* if $\det(\boldsymbol{W}) = +1$ and improper motions if $\det(\boldsymbol{W}) = -1$. Improper motions are called *inversions* if $\boldsymbol{W} = -\boldsymbol{I}$; *reflections* if $\boldsymbol{W}^2 = \boldsymbol{I}$ and $\boldsymbol{W} \neq -\boldsymbol{I}$; and *rotoinversions* in all other cases. The inversion is a rotation for spaces of even dimension, but an (improper) motion of its own kind in spaces of odd dimension. The origin is among the fixed points if $\boldsymbol{w} = \boldsymbol{o}$, where $\boldsymbol{o}$ is the $(n\times 1)$ column consisting entirely of zeros.

(3) *Fixed-point-free motions which are not translations.* In E^3, they are called *screw rotations* if $\det(\boldsymbol{W}) = +1$ and *glide reflections* if $\det(\boldsymbol{W}) = -1$. In E^2, only glide reflections occur. No such motions occur in E^1.

In Fig. 8.1.2.2, the relations between the different types of motions in E^3 are illustrated. The diagram contains all kinds of motions except the identity mapping I which leaves the whole space invariant and which is described by $\mathbb{W} = \mathbb{I}$. Thus, it is simultaneously a special rotation (with rotation angle 0) and a special translation (with translation vector $\mathbf{o}$).

So far, motions M in point space E^n have been considered. Motions give rise to mappings of the corresponding vector space $\mathbf{V}^n$ onto itself. If M maps the points P_1 and Q_1 of E^n onto P_2 and Q_2, the vector $\overrightarrow{P_1Q_1}$ is mapped onto the vector $\overrightarrow{P_2Q_2}$. If the motion in E^n is described by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, the vectors $\mathbf{v}$ of $\mathbf{V}^n$ are mapped according to $\tilde{\mathbf{v}} = \boldsymbol{W}\mathbf{v}$. In other words, of the linear and translation parts of the motion of E^n, only the linear part remains in the corresponding mapping of $\mathbf{V}^n$ (*linear mapping*). This difference between the mappings in the two spaces is particularly obvious for translations. For a translation T with translation vector $\mathbf{t} \neq \mathbf{o}$, no fixed point exists in E^n, *i.e.* no point of E^n is mapped onto itself by T. In $\mathbf{V}^n$, however, any vector $\mathbf{v}$ is mapped onto itself since the corresponding linear mapping is the identity mapping.

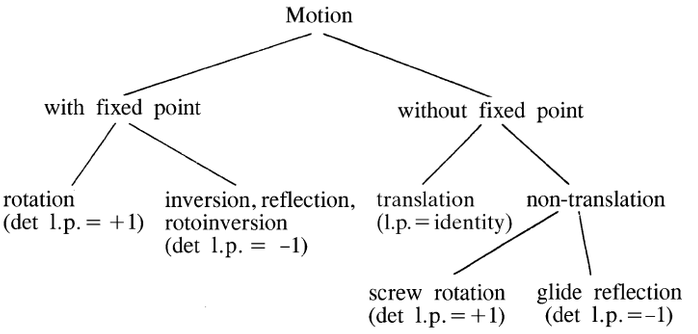

Fig. 8.1.2.2. Relations between the different kinds of motions in E^3; det l.p. = determinant of the linear part. The identity mapping does not fit into this scheme properly and hence has been omitted.

8.1.3. Symmetry operations and symmetry groups

Definition: A *symmetry operation* of a given object in point space E^n is a motion of E^n which maps this object (point, set of points, crystal pattern *etc.*) onto itself.

Remark: Any motion may be a symmetry operation, because for any motion one can construct an object which is mapped onto itself by this motion.

For the set of *all* symmetry operations of a given object, the following relations hold:

(*a*) successive application of two symmetry operations of an object results in a third symmetry operation of that object;

(*b*) the inverse of a symmetry operation is also a symmetry operation;

(*c*) there exists an 'identity operation' I which leaves each point of the space fixed: $X \rightarrow X$. This operation I is described (in any coordinate system) by $(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{o})$ or by $\mathbb{W} = \mathbb{I}$ and it is a symmetry operation of any object.

(*d*) The 'associative law' $(\mathsf{W}_3\mathsf{W}_2)\mathsf{W}_1 = \mathsf{W}_3(\mathsf{W}_2\mathsf{W}_1)$ is valid.

One can show, however, that in general the 'commutative law' $\mathsf{W}_2\mathsf{W}_1 = \mathsf{W}_1\mathsf{W}_2$ is not obeyed for symmetry operations.

The properties (*a*) to (*d*) are the group axioms. Thus, the set of all symmetry operations of an object forms a group, *the symmetry group of the object* or its *symmetry.* The mathematical theorems of *group theory*, therefore, may be applied to the symmetries of objects.

So far, only rather general objects have been considered. Crystallographers, however, are particularly interested in the symmetries of crystals. In order to introduce the concept of crystallographic symmetry operations, crystal structures, crystal patterns and lattices have to be taken into consideration. This will be done in the following section.

8.1.4. Crystal patterns, vector lattices and point lattices

Crystals are finite real objects in physical space which may be idealized by infinite three-dimensional periodic 'crystal structures' in point space. Three-dimensional periodicity means that there are translations among the symmetry operations of the object with the translation vectors spanning a three-dimensional space. Extending this concept of crystal structure to more general periodic objects and to n-dimensional space, one obtains the following definition:

Definition: An object in n-dimensional point space E^n is called an n-dimensional *crystallographic pattern* or, for short, *crystal pattern* if among its symmetry operations

(i) there are n translations, the translation vectors $\mathbf{t}_1, \ldots, \mathbf{t}_n$ of which are linearly independent,

(ii) all translation vectors, except the zero vector **o**, have a length of at least $d > 0$.

Condition (i) guarantees the n-dimensional periodicity and thus excludes subperiodic symmetries like layer groups, rod groups and frieze groups. Condition (ii) takes into account the finite size of atoms in actual crystals.

Successive application of two translations of a crystal pattern results in another translation, the translation vector of which is the (vector) sum of the original translation vectors. Consequently, in addition to the n linearly independent translation vectors $\mathbf{t}_1, \ldots, \mathbf{t}_n$, all (infinitely many) vectors $\mathbf{t} = u_1\mathbf{t}_1 + \ldots + u_n\mathbf{t}_n$ ($u_1, \ldots, u_n$ arbitrary integers) are translation vectors of the pattern. Thus, infinitely many translations belong to each crystal pattern. The periodicity of crystal patterns is represented by their lattices. It is useful to distinguish two kinds of lattices: vector lattices and point lattices. This distinction corresponds to that between vector space and point space, discussed above. The vector lattice is treated first.

Definition: The (infinite) set of *all* translation vectors of a crystal pattern is called the lattice of translation vectors or the *vector lattice* **L** of this crystal pattern.

In principle, any set of n linearly independent vectors may be used as a basis of the vector space $\mathbf{V}^n$. Most of these sets, however, result in a rather complicated description of a given vector lattice. The following theorem shows that among the (infinitely many) possible bases of the vector space $\mathbf{V}^n$ special bases always exist, referred to which the survey of a given vector lattice becomes particularly simple.

Definitions: (1) A basis of n vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$ of $\mathbf{V}^n$ is called a *crystallographic basis* of the n-dimensional vector lattice **L** if *every* integral linear combination $\mathbf{t} = u_1\mathbf{a}_1 + \ldots + u_n\mathbf{a}_n$ is a lattice vector of **L**. (2) A basis is called a primitive crystallographic basis of **L** or, for short, a *primitive basis* if it is a crystallographic basis and if, furthermore, *every* lattice vector **t** of **L** may be obtained as an *integral* linear combination of the basis vectors.

The distinction between these two kinds of bases can be expressed as follows. Referred to a crystallographic basis, the coefficients of each lattice vector must be either integral or rational. Referred to a primitive crystallographic basis, only integral coefficients occur. It should be noted that nonprimitive crystallographic bases are used conventionally for the description of 'centred lattices', whereas reduced bases are always primitive; see Chapter 9.2.

Example

The basis used conventionally for the description of the 'cubic body-centred lattice' is a crystallographic basis because the basis vectors **a**, **b**, **c** are lattice vectors. It is not a primitive basis because lattice vectors with non-integral but rational coefficients exist, *e.g.* the vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$. The bases $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$ or $\mathbf{a}'' = \mathbf{a}$, $\mathbf{b}'' = \mathbf{b}$, $\mathbf{c}'' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ are primitive bases. In the first of these bases, the vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ is given by $\mathbf{a}' + \mathbf{b}' + \mathbf{c}'$, in the second basis by $\mathbf{c}''$, both with integral coefficients only.

Fundamental theorem on vector lattices: For every vector lattice **L** primitive bases exist.

It can be shown that (in dimensions $n > 1$) the number of primitive bases for each vector lattice is infinite. There exists, however, a procedure called 'basis reduction' (*cf.* Chapter 9.2), which uniquely selects one primitive basis from this infinite set, thus permitting unambiguous description and comparison of vector lattices. Although such a reduced primitive basis always *can* be selected, in many cases conventional coordinate systems are chosen with nonprimitive rather than primitive crystallographic bases. The reasons are given in Section 8.3.1. The term 'primitive' is used not only for bases of lattices but also with respect to the lattices themselves, as in the crystallographic literature a *vector lattice* is frequently called *primitive* if its *conventional basis is primitive.*

With the help of the vector lattices defined above, the concept of point lattices will be introduced.

Definition: Given an arbitrary point X_0 in point space and a vector lattice **L** consisting of vectors $\mathbf{t}_j$, the set of all points X_j with $\overrightarrow{X_0X_j} = \mathbf{t}_j$ is called the *point lattice* belonging to X_0 and **L**.

A point lattice can be visualized as the set of end-points of all vectors of **L**, where **L** is attached to an arbitrary point X_0 of point space. Because each point X of point space could be chosen as the point X_0, an infinite set of point lattices belongs to each vector lattice. Frequently, the point X_0 is chosen as the origin of the coordinate system of the point space.

An important aspect of a lattice is its *unit cell*.

Definition: If $\mathbf{a}_1, \ldots, \mathbf{a}_n$ is a crystallographic basis of a vector lattice **L**, the set of all vectors $x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ with $0 \leq x_i < 1$ is called a *unit cell of the vector lattice.*

The concept of a 'unit cell' is not only applied to vector lattices in vector space but also more often to crystal structures or crystal patterns in point space. Here the coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ and the origin X_0 of the unit cell have to be chosen. In most cases $X_0 = O$ is taken, but in general we have the following definition:

Definition: Given a crystallographic coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$ of a crystal pattern and a point X_0 with coordinates x_{0i}, a *unit cell of the crystal pattern* is the set of all points X with coordinates x_i such that the equation $0 \leq x_i - x_{0i} < 1$ $(i = 1, \ldots, n)$ holds.

Obviously, the term 'unit cell' may be transferred to real crystals. As the volume of the unit cell and the volumes of atoms are both finite, only a *finite* number N of atoms can occur in a unit cell of a crystal. A crystal structure, therefore, may be described in two ways:

(*a*) One starts with an arbitrary unit cell and builds up the whole crystal structure by infinite repetition of this unit cell. The crystal structure thus consists of an infinite number of finite 'building blocks', each building block being a unit cell.

(*b*) One starts with a point X_1 representing the centre of an atom. To this point belong an infinite number of translationally equivalent points X_j, *i.e.* points for which the vectors $\overrightarrow{X_1X_j}$ are lattice vectors. In this way, from each of the points X_i $(i = 1, \ldots, N)$ within the unit cell a point lattice of translationally equivalent points is obtained. The crystal structure is then described by a finite number of interpenetrating infinite point lattices.

In most cases, one is not interested in the orientation of the vector lattice or the point lattices of a crystal structure in space, but only in the shape and size of a unit cell. From this point of view, a three-dimensional lattice is fully described by the lengths a, b and c of the basis vectors **a**, **b** and **c** and by the three interaxial angles α, β and γ. These data are called the *lattice parameters*, *cell parameters* or *lattice constants* of both the vector lattice and the associated point lattices of the crystal structure.

8.1.5. Crystallographic symmetry operations

Crystallographic symmetry operations are special motions.

Definition: A motion is called a *crystallographic symmetry operation* if a crystal pattern exists for which it is a symmetry operation.

We consider a crystal pattern with its vector lattice $\mathbf{L}$ referred to a primitive basis. Then, by definition, each vector of $\mathbf{L}$ has integral coefficients. The linear part of a symmetry operation maps $\mathbf{L}$ onto itself: $\mathbf{L} \rightarrow \boldsymbol{W}\mathbf{L} = \mathbf{L}$. Since the coefficients of all vectors of $\mathbf{L}$ are integers, the matrix $\boldsymbol{W}$ is an integral matrix, *i.e.* its coefficients are integers. Thus, the trace of $\boldsymbol{W}$, $\mathrm{tr}(\boldsymbol{W}) = \boldsymbol{W}_{11} + \ldots + \boldsymbol{W}_{nn}$, is also an integer. In $\mathbf{V}^3$, by reference to an appropriate orthonormal (not necessarily crystallographic) basis, one obtains another condition for the trace, $\mathrm{tr}(\boldsymbol{W}) = \pm(1 + 2\cos\varphi)$, where φ is the angle of rotation or rotoinversion. From these two conditions, it follows that φ can only be 0, 60, 90, 120, 180° *etc.*, and hence the familiar restriction to one-, two-, three-, four- and sixfold rotations and rotoinversions results.* These results imply for dimensions 2 and 3 that the matrix $\boldsymbol{W}$ satisfies the condition $(\boldsymbol{W})^{\boldsymbol{k}} = \boldsymbol{I}$, with $k = 1, 2, 3, 4$ or 6.† Consequently, for the operation $(\boldsymbol{W}, \boldsymbol{w})$ in point space the relation

$$(\boldsymbol{W},\boldsymbol{w})^{\boldsymbol{k}} = [\boldsymbol{I}, (\boldsymbol{W}^{\boldsymbol{k-1}} + \boldsymbol{W}^{\boldsymbol{k-2}} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w}] = (\boldsymbol{I},\boldsymbol{t})$$

holds.

For the motion described by $(\boldsymbol{W}, \boldsymbol{w})$, this implies that a k-fold application results in a translation T (with translation vector $\mathbf{t}$) of the crystal pattern. The (fractional) translation $(1/k)\mathsf{T}$ is called the *intrinsic translation part* (*screw or glide part*) of the symmetry operation. Whereas the 'translation part' of a motion depends on the choice of the origin, the 'intrinsic translation part' of a motion is uniquely determined. The intrinsic translation vector $(1/k)\mathbf{t}$ is the shortest translation vector of the motion for any choice of the origin.

If $\boldsymbol{t} = \boldsymbol{o}$, the symmetry operation has at least one fixed point and is a rotation, inversion, reflection or rotoinversion. If $\boldsymbol{t} \neq \boldsymbol{o}$, the term $(1/k)\mathbf{t}$ is called the *glide vector* (for a reflection) or the *screw vector* (for a rotation) of the symmetry operation. Both types of operations, glide reflections and screw rotations, have no fixed point.

For the geometric visualization of symmetry, the concept of *symmetry elements* is useful.‡ The symmetry element of a symmetry operation is the set of its fixed points, together with a characterization of the motion. For symmetry operations without fixed points (screw rotations or glide reflections), the fixed points of the corresponding rotations or reflections, described by $(\boldsymbol{W}, \boldsymbol{w}')$ with $\boldsymbol{w}' = \boldsymbol{w} - (1/k)\boldsymbol{t}$, are taken. Thus, in E^2, symmetry elements are N-fold rotation points ($N = 2$, 3, 4 or 6), mirror lines and glide lines. In E^3, symmetry elements are rotation axes, screw axes, inversion centres, mirror planes and glide planes. A peculiar situation exists for rotoinversions (except $\bar{1}$ and $\bar{2} \equiv m$). The symmetry element of such a rotoinversion consists of two components, a point and an axis. The point is the *inversion point* of the rotoinversion, and the *axis* of the rotoinversion is that of the corresponding rotation.

The determination of both the nature of a symmetry operation and the location of its symmetry element from the coordinate triplets, listed under *Positions* in the space-group tables, is described in Section 11.2.1 of Chapter 11.2.

8.1.6. Space groups and point groups

As mentioned in Section 8.1.3, the set of all symmetry operations of an object forms a group, the symmetry group of that object.

Definition: The symmetry group of a three-dimensional crystal pattern is called its *space group*. In E^2, the symmetry group of a (two-dimensional) crystal pattern is called its *plane group*. In E^1, the symmetry group of a (one-dimensional) crystal pattern is called its *line group*. To each crystal pattern belongs an infinite set of translations T_j which are symmetry operations of that pattern. The set of all T_j forms a group known as the *translation subgroup* $\mathcal{T}$ of the space group $\mathcal{G}$ of the crystal pattern. Since the commutative law $\mathsf{T}_j\mathsf{T}_k = \mathsf{T}_k\mathsf{T}_j$ holds for any two translations, $\mathcal{T}$ is an Abelian group. With the aid of the translation subgroup $\mathcal{T}$, an insight into the architecture of the space group $\mathcal{G}$ can be gained.

Referred to a coordinate system $(O, \mathbf{a}_1, \ldots, \mathbf{a}_n)$, the space group $\mathcal{G}$ is described by the set $\{(\boldsymbol{W}, \boldsymbol{w})\}$ of matrices $\boldsymbol{W}$ and columns $\boldsymbol{w}$. The group $\mathcal{T}$ is represented by the set of elements $(\boldsymbol{I}, \boldsymbol{t}_j)$, where $\boldsymbol{t}_j$ are the columns of coefficients of the translation vectors $\mathbf{t}_j$ of the lattice $\mathbf{L}$. Let $(\boldsymbol{W}, \boldsymbol{w})$ describe an arbitrary symmetry operation W of $\mathcal{G}$. Then, all products $(\boldsymbol{I}, \boldsymbol{t}_j)(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t}_j)$ for the different j have the same matrix part $\boldsymbol{W}$. Conversely, every symmetry operation W of the space group with the same matrix part $\boldsymbol{W}$ is represented in the set $\{(\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t}_j)\}$. The corresponding set of symmetry operations can be denoted by $\mathcal{T}\mathsf{W}$. Such a set is called a *right coset of $\mathcal{G}$ with respect to $\mathcal{T}$*, because the element W is the right factor in the products $\mathcal{T}\mathsf{W}$. Consequently, the space group $\mathcal{G}$ may be decomposed into the right cosets $\mathcal{T}, \mathcal{T}\mathsf{W}_2, \mathcal{T}\mathsf{W}_3, \ldots, \mathcal{T}\mathsf{W}_i$, where the symmetry operations of the same column have the same matrix part $\boldsymbol{W}$, and the symmetry operations W_j differ by their matrix parts $\boldsymbol{W}_j$. This *coset decomposition of $\mathcal{G}$ with respect to $\mathcal{T}$* may be displayed by the array

$\mathsf{I} \equiv \mathsf{W}_1$	W_2	W_3	...	W_i
T_1	$\mathsf{T}_1\mathsf{W}_2$	$\mathsf{T}_1\mathsf{W}_3$	...	$\mathsf{T}_1\mathsf{W}_i$
T_2	$\mathsf{T}_2\mathsf{W}_2$	$\mathsf{T}_2\mathsf{W}_3$	...	$\mathsf{T}_2\mathsf{W}_i$
T_3	$\mathsf{T}_3\mathsf{W}_2$	$\mathsf{T}_3\mathsf{W}_3$	...	$\mathsf{T}_3\mathsf{W}_i$
⋮	⋮	⋮		⋮

Here, $\mathsf{W}_1 = \mathsf{I}$ is the identity operation and the elements of $\mathcal{T}$ form the first column, those of $\mathcal{T}\mathsf{W}_2$ the second column *etc.* As each column may be represented by the common matrix part $\boldsymbol{W}$ of its symmetry operations, the number i of columns, *i.e.* the number of cosets, is at the same time the number of *different* matrices $\boldsymbol{W}$ of the symmetry operations of $\mathcal{G}$. This number i is always finite, and is the order of the point group belonging to $\mathcal{G}$, as explained below. Any element of a coset $\mathcal{T}\mathsf{W}_j$ may be chosen as the representative element of that coset and listed at the top of its column. Choice of a different representative element merely results in a different order of the elements of a coset, but the coset does not change its content.§

Analogously, a coset $\mathsf{W}\mathcal{T}$ is called a *left coset* of $\mathcal{G}$ with respect to $\mathcal{T}$, and $\mathcal{G}$ can be decomposed into the left cosets $\mathcal{T}, \mathsf{W}_2\mathcal{T}, \mathsf{W}_3\mathcal{T}, \ldots, \mathsf{W}_i\mathcal{T}$. This left coset decomposition of a space group is always possible with the same $\mathsf{W}_1, \mathsf{W}_2, \ldots, \mathsf{W}_i$ as in the right coset decomposition. Moreover, both decompositions result in the same cosets, except for the order of the elements in each coset. A subgroup of a group with these properties is called a *normal subgroup* of the group; *cf.* Ledermann (1976). Thus, the translation subgroup $\mathcal{T}$ is a normal subgroup of the space group $\mathcal{G}$.

The decomposition of a space group into cosets is the basis of the description of the space groups in these *Tables*. The symmetry

* The reflection $m \equiv \bar{2}$ is contained among the rotoinversions. The same restriction is valid for the rotation angle φ in two-dimensional space, where $\mathrm{tr}(\boldsymbol{W}) = 2\cos\varphi$ if $\det(\boldsymbol{W}) = +1$. If $\det(\boldsymbol{W}) = -1$, $\mathrm{tr}(\boldsymbol{W}) = 0$ always holds and the operation is a reflection m.

† A method of deriving the possible orders of $\boldsymbol{W}$ in spaces of arbitrary dimension has been described by Hermann (1949).

‡ For a rigorous definition of the term *symmetry element*, see de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000).

§ A coset decomposition of a group $\mathcal{G}$ is possible with respect to every subgroup $\mathcal{H}$ of $\mathcal{G}$; *cf.* Ledermann (1976). The number of cosets is called the *index* $[i]$ of $\mathcal{H}$ in $\mathcal{G}$. The integer $[i]$ may be finite, as for the coset decomposition of a space group $\mathcal{G}$ with respect to the (infinite) translation group $\mathcal{T}$ or infinite, as for the coset decomposition of a space group $\mathcal{G}$ with respect to a (finite) site-symmetry group $\mathcal{S}$; *cf.* Section 8.3.2. If $\mathcal{G}$ is a finite group, a theorem of Lagrange states that the order of $\mathcal{G}$ is the product of the order of $\mathcal{H}$ and the index of $\mathcal{H}$ in $\mathcal{G}$.

operations of the space group are referred to a 'conventional' coordinate system (*cf.* Section 8.3.1) and described by $(n+1) \times (n+1)$ matrices. In the space-group tables as *general position* (*cf.* Section 8.3.2) for each column, a representative is listed whose coefficients w_j obey the condition $0 \leq w_j < 1$. The matrix is not listed completely, however, but is given in a short-hand notation. In the expression $W_{j1}x_1 + \ldots + W_{jn}x_n + w_j$, all vanishing terms and all $W_{jk} = 1$ are omitted, *e.g.*

$$\left.\begin{array}{l} 1x + 0y + 0z + \frac{1}{2} \\ 0x + 1y + 0z + 0 \\ 0x + 0y - 1z + \frac{1}{2} \end{array}\right\}$$

is replaced by $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$. The first entry of the general position is always the identity mapping, listed as x, y, z. It represents all translations of the space group too.

As groups, some space groups are more complicated than others. Most easy to survey are the 'symmorphic' space groups which may be defined as follows:

Definition: A space group is called *symmorphic* if the coset representatives W_j can be chosen in such a way that they leave one common point fixed.

In this case, the representative symmetry operations W_j of a symmorphic space group form a (finite) group. If the fixed point is chosen as the origin of the coordinate system, the column parts $\boldsymbol{w}_j$ of the representative symmetry operations W_j obey the equations $\boldsymbol{w}_j = \boldsymbol{o}$. Thus, for a symmorphic space group the representative symmetry operations may always be described by the special matrix–column pairs $(\boldsymbol{W}_j, \boldsymbol{o})$.

Symmorphic space groups may be easily identified by their Hermann–Mauguin symbols because these do not contain any glide or screw operation. For example, the monoclinic space groups with the symbols $P2$, $C2$, Pm, Cm, $P2/m$ and $C2/m$ are symmorphic, whereas those with the symbols $P2_1$, Pc, Cc, $P2_1/m, P2/c, P2_1/c$ and $C2/c$ are not.

Unlike most textbooks of crystallography, in this section point groups are treated after space groups because the space group of a crystal pattern, and thus of a crystal structure, determines its point group uniquely.

The external shape (morphology) of a macroscopic crystal is formed by its faces. In order to eliminate the influence of growth conditions, the set of crystal faces is replaced by the set of face normals, *i.e.* by a set of vectors. Thus, the symmetry group of the macroscopic crystal is the symmetry group of the *vector set of face normals*. It is not the group of motions in point space, therefore, that determines the symmetry of the macroscopic crystal, but the corresponding group of linear mappings of vector space; *cf.* Section 8.1.2. This group of linear mappings is called the *point group of the crystal.* Since to each macroscopic crystal a crystal structure corresponds and, furthermore, to each crystal structure a space group, the point group of the crystal defined above is also the point group of the crystal structure and the point group of its space group.

To connect more formally the concept of point groups with that of space groups in n-dimensional space, we consider the coset decomposition of a space group $\mathcal{G}$ with respect to the normal subgroup $\mathcal{T}$, as displayed above. We represent the right coset decomposition by $\mathcal{T}, \mathcal{T}\mathsf{W}_2, \ldots, \mathcal{T}\mathsf{W}_i$ and the corresponding left coset decomposition by $\mathcal{T}, \mathsf{W}_2\mathcal{T}, \ldots, \mathsf{W}_i\mathcal{T}$. If $\mathcal{G}$ is referred to a coordinate system, the symmetry operations of $\mathcal{G}$ are described by matrices $\boldsymbol{W}$ and columns $\boldsymbol{w}$. As a result of the one-to-one correspondence between the i cosets $\mathcal{T}\mathsf{W}_j = \mathsf{W}_j\mathcal{T}$ and the i matrices $\boldsymbol{W}_j$, the cosets may alternatively be represented by the matrices $\boldsymbol{W}_j$. These matrices form a group of (finite) order i, and they describe linear mappings of the vector space $\mathbf{V}^n$ connected with E^n; *cf.* Section 8.1.2. This group (of order i) of linear mappings is the *point group $\mathcal{P}$ of the space group $\mathcal{G}$*, introduced above.

The difference between symmetry in point space and that in vector space may be exemplified again by means of some monoclinic space groups. Referred to conventional coordinate systems, space groups Pm, Pc, Cm and Cc have the same (3×3) matrices $\boldsymbol{W}_j$ of their symmetry operations. Thus, the point groups of all these space groups are of the same type *m.* The space groups themselves, however, show a rather different behaviour. In Pm and Cm reflections occur, whereas in Pc and Cc only glide reflections are present.

Remark: The usage of the term 'point group' in connection with space groups is rather unfortunate as the *point group of a space group* is *not* a group of motions of *point space* but a group acting on *vector space.* As a consequence, the point group of a space group may contain operations which do not occur in the space group at all. This is apparent from the example of monoclinic space groups above. Nevertheless, the term 'point group of a space group' is used here for historical reasons. A more adequate term would be 'vector point group' of a space group or a crystal. It must be mentioned that the term 'point group' is also used for the 'site-symmetry group', defined in Section 8.3.2. Site-symmetry groups are groups acting on point space.

It is of historic interest that the 32 types of three-dimensional crystallographic point groups were determined more than 50 years before the 230 (or 219) types of space group were known. The physical methods of the 19th century, *e.g.* the determination of the symmetry of the external shape or of tensor properties of a crystal, were essentially methods of determining the point group, not the space group of the crystal.

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