(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 $\mathcal{G}$.