International Tables for Crystallography (2011). Vol. A1, Section 1.2.5, pp. 14–18.

normal subgroup of $\mathcal{G}$, there may nevertheless be elements $g_p \in \mathcal{G}$, $g_p \notin \mathcal{H}$ for which $g_p^{-1}\mathcal{H}g_p = \mathcal{H}$ holds. We consider the set of all elements $g_p \in \mathcal{G}$ that have this property.

Definition 1.2.4.5.1. The set of all elements $g_p \in \mathcal{G}$ that map the subgroup $\mathcal{H} < \mathcal{G}$ onto itself by conjugation, $\mathcal{H} = g_p^{-1}\mathcal{H}g_p = \mathcal{H}^{g_p}$, forms a group $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$, called the *normalizer of* $\mathcal{H}$ *in* $\mathcal{G}$, where $\mathcal{H} \trianglelefteq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$. □

Remarks

(1) The group $\mathcal{H} < \mathcal{G}$ is a normal subgroup of $\mathcal{G}$, $\mathcal{H} \triangleleft \mathcal{G}$, if and only if $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$.

(2) Let $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \{g_p\}$. One can decompose $\mathcal{G}$ into right cosets relative to $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. All elements $g_p\, g_r$ of a right coset $\mathcal{N}_{\mathcal{G}}(\mathcal{H})\, g_r$ of this decomposition $(\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H}))$ transform $\mathcal{H}$ into the same subgroup $g_r^{-1}\, g_p^{-1}\, \mathcal{H}\, g_p\, g_r = g_r^{-1}\, \mathcal{H}\, g_r < \mathcal{G}$, which is thus conjugate to $\mathcal{H}$ in $\mathcal{G}$ by g_r.

(3) The elements of different cosets of $(\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H}))$ transform $\mathcal{H}$ into different conjugates of $\mathcal{H}$. The number of cosets of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ is equal to the index $i_N = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$ of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ in $\mathcal{G}$. Therefore, the number $N_{\mathcal{H}}$ of conjugates in the conjugacy class of $\mathcal{H}$ is equal to the index i_N and is thus determined by the order of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. From $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) \geq \mathcal{H}$, $i_N = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})| \leq |\mathcal{G} : \mathcal{H}| = i$ follows. This means that the number of conjugates of a subgroup $\mathcal{H} < \mathcal{G}$ cannot exceed the index $i = |\mathcal{G} : \mathcal{H}|$.

(4) If $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of $\mathcal{G}$, then either $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{G}$ and $\mathcal{H} \triangleleft \mathcal{G}$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{H}$ and the number of conjugates is equal to the index $i = |\mathcal{G} : \mathcal{H}|$.

(5) For the normalizers of the space groups, see the corresponding part of Section 1.2.6.3.

1.2.5. Space groups

1.2.5.1. Space groups and their description

The set of all symmetry operations of a three-dimensional crystal pattern, *i.e.* its symmetry group, is the *space group* of this crystal pattern. In a plane, the symmetry group of a two-dimensional crystal pattern is its *plane group*. In the following, the term 'space group' alone will be used and the plane groups are included because they are the space groups of two-dimensional space.

A crystal pattern is a periodic array. This means that there are translations among its symmetry operations. The translations of crystals are small (up to a few hundred ångströms) but cannot be arbitrarily short because of the finite size of the particles in crystal structures. One thus defines for any finite integer n:

Definition 1.2.5.1.1. A group $\mathcal{G}$ of isometries in n-dimensional space is called an n-dimensional space group if

(1) $\mathcal{G}$ contains n linearly independent translations.

(2) There is a minimum length $\delta > 0$ such that the length r of any translation vector is at least $r = \delta$. □

Condition (2) is justified because crystal structures contain atoms of finite size, and it is necessary to avoid infinitely small translations as elements of space groups. Several fundamental properties would not hold without this condition, such as the existence of a lattice of translation vectors and the restriction to only a few rotation angles.

In this volume, only the dimensions $n = 2$ and $n = 3$ will be dealt with. However, the space groups (more precisely, the space-group types, *cf.* Section 1.2.5.3) and other crystallographic items are also known for dimensions n = 4, 5 and 6. For example, the number of affine space-group types for n = 6 is 28 927 922 (Plesken & Schulz, 2000). 7052 of these affine space-group types split into enantiomorphic pairs of space groups, such that there are 28 934 974 crystallographic space-group types (Souvignier, 2003).

One of the characteristics of a space group is its translation group. Any space group $\mathcal{G}$ is an infinite group because the number of its translations is already infinite. The set of all translations of $\mathcal{G}$ forms the infinite translation subgroup $\mathcal{T}(\mathcal{G}) \triangleleft \mathcal{G}$ with the composition law of performing one translation after the other, represented by the multiplication of matrix–column pairs. The group $\mathcal{T}(\mathcal{G})$ is a normal subgroup of $\mathcal{G}$ of finite index. The vector lattice **L**, *cf.* Section 1.2.2.2, forms a group with the composition law of vector addition. This group is isomorphic to the group $\mathcal{T}(\mathcal{G})$.

The matrix–column pairs of the symmetry operations of a space group $\mathcal{G}$ are mostly referred to the *conventional coordinate system*. Its basis is chosen as a lattice basis and in such a way that the matrices for the linear parts of the symmetry operations of $\mathcal{G}$ are particularly simple. The origin is chosen such that as many coset representatives as possible can be selected with their column coefficients to be zero, or such that the origin is situated on a centre of inversion. This means (for details and examples see Section 8.3.1 of *IT* A):

(1) The basis is always chosen such that all matrix coefficients are 0 or ±1.

(2) If possible, the basis is chosen such that all matrices have main diagonal form; then six of the nine coefficients are 0 and three are ±1.

(3) If (2) is not possible, the basis is chosen such that the matrices are orthogonal. Again, six coefficients are 0 and three are ±1.

(4) If (3) is not possible, the basis is hexagonal. At least five of the nine matrix coefficients are 0 and at most four are ±1.

(5) The conventional basis chosen according to these rules is not always primitive, *cf.* the first example of Section 8.3.1 of *IT* A. If the conventional basis is primitive, then the lattice is also called *primitive*; if the conventional basis is not primitive, then the lattice referred to this (non-primitive) basis is called a *centred lattice*.

(6) The matrix parts of a translation and of an inversion are

$$\boldsymbol{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \bar{\boldsymbol{I}} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix},$$

i.e. the unit matrix and the negative unit matrix. They are independent of the basis.

(7) The basis vectors of a crystallographic basis are lattice vectors. This makes the description of the lattice and of the symmetry operations of a crystal pattern independent of the actual metrics of the lattice, for example independent of temperature and pressure. It also means that the description of the symmetry may be the same for space groups of the same type, *cf.* Section 1.2.5.3.

(8) The origin is chosen at a point of highest site symmetry which is left invariant by as many symmetry operations as possible. The column parts $\boldsymbol{w}_k$ of these symmetry operations are $\boldsymbol{w}_k = \boldsymbol{o}$, *i.e.* the columns consist of zeroes only.

It is obviously impossible to list all elements of an infinite group individually. One can define the space group by a set of generators, because the number of necessary generators for any space group is finite: theoretically, up to six generators might be necessary but in practice up to ten generators are chosen for a space group. In *IT* A and in this volume, the set of the conventional generators is listed in the block 'Generators selected'. The unit element is taken as the first generator; the generating translations follow and the generation is completed with the generators of the non-translational symmetry operations. The rules for the choice of the conventional generators are described in *IT* A, Section 8.3.5.

The description by generators is particularly important for this volume because many of the maximal subgroups in Chapters 2.2 and 2.3 are listed by their generators. These generators are chosen such that the generation of the general position can follow a *composition series*, *cf.* Ledermann (1976) and Ledermann & Weir (1996). This procedure allows the generation by a short program or even by hand. For details see *IT* A, Section 8.3.5; in Table 8.3.5.2 of *IT* A an example for the generation of a space group along these lines is displayed.

There are four ways to describe a space group in *IT* A:

(i) A set of generators is the first way in which the space-group types $\mathcal{G}$, *cf.* Section 1.2.5.3, are described in *IT* A. This way is also used in the tables of this volume.
(ii) By the matrices of the coset representatives of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ in the general position. These matrices are not written in full but in a shorthand notation, *cf.* Section 8.1.5 or Chapter 11.1 of *IT* A. This kind of description is used for *translationengleiche* maximal subgroups in Chapters 2.2 and 2.3 of this volume, but in a slightly modified way, *cf.* Section 2.1.3.
(iii) In a visual way by diagrams of the symmetry elements (not symmetry operations!) of $\mathcal{G}$ within a unit cell and its surroundings.
(iv) Also in a visual way by depicting the general-position points, again within a unit cell and its surroundings.

1.2.5.2. Classifications of space groups

There are an infinite number of space groups because there are an infinite number of known or conceivable crystals and crystal patterns. Indeed, because the lattice parameters depend on temperature and pressure, so do the lattice translations and the space group of a crystal. There is great interest in getting an overview of this vast number of space groups. To achieve this goal, one first characterizes the space groups by their group-theoretical properties and classifies them into space-group types where the space groups of each type have certain properties in common. To get a better overview, one then classifies the space-group types such that related types belong to the same 'super-class'. This classification is done in two ways (*cf.* Sections 1.2.5.4 and 1.2.5.5):

(1) first into *geometric crystal classes* by the point group of the space group, and then into *crystal systems*;
(2) into the arithmetic crystal classes of the space groups and then into *Bravais flocks* and into *lattice systems* (not treated here, *cf. IT* A, Section 8.2.5);
(3) all these classes: geometric and arithmetic crystal classes, crystal systems, Bravais flocks and lattice systems are classified into *crystal families.*

In reality, the tables in Chapters 2.2 and 2.3 and the graphs in Chapters 2.4 and 2.5 are tables and graphs for space-group types. The sequence of the space-group types in *IT* A and thus in this volume is determined by their crystal class, their crystal system and their crystal family. Therefore, these classifications are treated in the next sections. The point groups and the translation groups of the space groups can also be classified in a similar way. Only the classification of the point groups is treated in this chapter. For a more detailed treatment and for the classification of the lattices, the reader is referred to Chapter 1.4 of this volume, to Part 8 of *IT* A or to Brown *et al.* (1978).

1.2.5.3. Space groups and space-group types

We first consider the classification of the space groups into types. A more detailed treatment may be found in Section 8.2.1 of *IT* A. In practice, a common way is to look for the symmetry of the space group $\mathcal{G}$ and to compare this symmetry with that of the diagrams in the tables of *IT* A.

With the exception of some double descriptions,[6] there is exactly one set of diagrams which displays the symmetry of $\mathcal{G}$, and $\mathcal{G}$ belongs to that space-group type which is described in this set. From those diagrams the Hermann–Mauguin symbol, abbreviated as HM symbol, the Schoenflies symbol and the space-group number are taken.

A rigorous definition is:

Definition 1.2.5.3.1. Two space groups belong to the same *affine space-group type* if and only if they are isomorphic.[7] □

This definition refers to a rather abstract property which is of great mathematical but less practical value. In crystallography another definition is more appropriate which results in exactly the same space-group types as are obtained by isomorphism. It starts from the description of the symmetry operations of a space group by matrix–column pairs or, as will be formulated here, by augmented matrices. For this one refers each of the space groups to one of its lattice bases.

Definition 1.2.5.3.2. Two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same *affine space-group type* if for a lattice basis and an origin of $\mathcal{G}$, a lattice basis and an origin of $\mathcal{G}'$ can also be found so that the groups of augmented matrices $\{\mathbb{W}\}$ describing $\mathcal{G}$ and $\{\mathbb{W}'\}$ describing $\mathcal{G}'$ are identical. □

In this definition the coordinate systems are chosen such that the groups of augmented matrices agree. It is thus possible to describe the symmetry of all space groups of the same type by one (standardized) set of matrix–column pairs, as is done, for example, in the tables of *IT* A.

In the subgroup tables of Chapters 2.2 and 2.3 it frequently happens that a subgroup $\mathcal{H} < \mathcal{G}$ of a space group $\mathcal{G}$ is given by its matrix–column pairs referred to a nonconventional coordinate system. In this case, a transformation of the coordinate system can bring the matrix–column pairs to the standard form by which the space-group type may be determined. In the subgroup tables both the space-group type and the transformation of the coordinate system are listed. One can also use this procedure for the definition of the term 'affine space-group type':

Definition 1.2.5.3.3. Let two space groups $\mathcal{G}$ and $\mathcal{G}'$ be referred to lattice bases and represented by their groups of augmented matrices $\{\mathbb{W}\}$ and $\{\mathbb{W}'\}$. The groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same

[6] Monoclinic space groups are described in the settings 'unique axis *b*' and 'unique axis *c*'; rhombohedral space groups are described in the settings 'hexagonal axes' and 'rhombohedral axes'; and 24 space groups are described with two origins by 'origin choice 1' and 'origin choice 2'. In each case, both descriptions lead to the same short Hermann–Mauguin symbol and space-group number.

[7] The name 'affine space-group type' stems from Definition 1.2.5.3.3. 'Affine space-group types' have to be distinguished from 'crystallographic space-group types' which are defined by Definition 1.2.5.3.4.

affine space-group type if an augmented matrix $\mathbb{P}$ with linear part $\boldsymbol{P}$, $\det(\boldsymbol{P}) \neq 0$, and column part $\boldsymbol{p}$ exists, for which

$$\{\mathbb{W}'\} = \mathbb{P}^{-1}\{\mathbb{W}\}\,\mathbb{P} \qquad (1.2.5.1)$$

holds. □

The affine space-group types are classes in the mathematical sense of the word, *i.e.* each space group belongs to exactly one type. The derivation of these types reveals 219 affine space-group types and 17 plane-group types.

In crystallography one usually distinguishes 230 rather than 219 space-group types in a slightly finer subdivision. The difference can best be explained using Definition 1.2.5.3.3. The matrix part $\boldsymbol{P}$ may have a negative determinant. In this case, a right-handed basis is converted into a left-handed one, and right-handed and left-handed screw axes are exchanged. It is a convention in crystallography to always refer the space to a right-handed basis and hence transformations with $\det(\boldsymbol{P}) < 0$ are not admitted.

Definition 1.2.5.3.4. If the matrix $\boldsymbol{P}$ is restricted by the condition $\det(\boldsymbol{P}) > 0$, eleven affine space-group types split into two space-group types each, one with right-handed and one with left-handed screw axes, such that the total number of types is 230. These 230 space-group types are called *crystallographic space-group types*. The eleven splitting space-group types are called *pairs of enantiomorphic space-group types* and the space groups themselves are enantiomorphic pairs of space groups. □

The space groups of an enantiomorphic pair belong to different crystallographic space-group types but are isomorphic. As a consequence, in the lists of isomorphic subgroups $\mathcal{H} < \mathcal{G}$ of the tables of Chapter 2.3, there may occur subgroups $\mathcal{H}$ with another conventional HM symbol and another space-group number than that of $\mathcal{G}$, *cf.* Example 1.2.6.2.7. In such a case, $\mathcal{G}$ and $\mathcal{H}$ are members of an enantiomorphic pair of space groups and $\mathcal{H}$ belongs to the space-group type enantiomorphic to that of $\mathcal{G}$. There are no enantiomorphic pairs of plane groups.

The space groups are of different complexity. The simplest ones are the symmorphic space groups (not to be confused with 'isomorphic' space groups) according to the following definition:

Definition 1.2.5.3.5. A space group $\mathcal{G}$ is called *symmorphic* if representatives g_k of all cosets $\mathcal{T}(\mathcal{G})\,g_k$ can be found such that the set $\{g_k\}$ of all representatives forms a group. □

The group $\{g_k\}$ is finite and thus leaves a point F fixed. In the standard setting of any symmorphic space group such a point F is chosen as the origin. Thus, the translation parts of the elements g_k consist of zeroes only.

If a space group is symmorphic then all space groups of its type are symmorphic. Therefore, one can speak of 'symmorphic space-group types'. Symmorphic space groups can be recognized easily by their HM symbols: they contain an unmodified point-group symbol: rotations, reflections, inversions and rotoinversions but no screw rotations or glide reflections. There are 73 symmorphic space-group types of dimension three and 13 of dimension two; none of them show enantiomorphism.

One frequently speaks of 'the 230 space groups' or 'the 17 plane groups' and does not distinguish between the terms 'space group' and 'space-group type'. This is very often possible and is also done in this volume in order to make the explanations less long-winded. However, occasionally the distinction is indispensable in order to avoid serious difficulties of comprehension. For example, the sentence 'A space group is a proper subgroup of itself' is incomprehensible, whereas the sentence 'A space group and its proper subgroup belong to the same space-group type' makes sense.

1.2.5.4. Point groups and crystal classes

If the point coordinates are mapped by an isometry and its matrix–column pair, the vector coefficients are mapped by the linear part, *i.e.* by the matrix alone, *cf.* Section 1.2.2.6. Because the number of its elements is infinite, a space group generates from one point an infinite set of symmetry-equivalent points by its matrix–column pairs. Because the number of matrices of the linear parts is finite, the group of matrices generates from one vector a finite set of symmetry-equivalent vectors, for example the vectors normal to certain planes of the crystal. These planes determine the morphology of the ideal macroscopic crystal and its cleavage; the centre of the crystal represents the zero vector. When the symmetry of a crystal can only be determined by its macroscopic properties, only the symmetry group of the macroscopic crystal can be found. All its symmetry operations leave at least one point of the crystal fixed, *viz* its centre of mass. Therefore, this symmetry group was called the *point group of the crystal*, although its symmetry operations are those of vector space, not of point space. Although misunderstandings are not rare, this name is still used in today's crystallography for historical reasons.[8]

Let a conventional coordinate system be chosen and the elements $g_j \in \mathcal{G}$ be represented by the matrix–column pairs $(\boldsymbol{W}_j, \boldsymbol{w}_j)$, with the representation of the translations $t_k \in \mathcal{T}(\mathcal{G})$ by the pairs $(\boldsymbol{I}, \boldsymbol{t}_k)$. Then the composition of $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ with all translations forms an infinite set $\{(\boldsymbol{I}, \boldsymbol{t}_k)(\boldsymbol{W}_j, \boldsymbol{w}_j) = (\boldsymbol{W}_j, \boldsymbol{w}_j + \boldsymbol{t}_k)\}$ of symmetry operations which is a right coset of the coset decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$. From this equation it follows that the elements of the same coset of the decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ have the same linear part. On the other hand, elements of different cosets have different linear parts if $\mathcal{T}(\mathcal{G})$ contains all translations of $\mathcal{G}$. Thus, each coset can be characterized by its linear part. It can be shown from equations (1.2.2.5) and (1.2.2.6) that the linear parts form a group which is isomorphic to the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, *i.e.* to the group of the cosets.

Definition 1.2.5.4.1. A group of linear parts, represented by a group of matrices $\boldsymbol{W}_j$, is called a *point group* $\mathcal{P}$. If the linear parts are those of the matrix–column pairs describing the symmetry operations of a space group $\mathcal{G}$, the group is called the *point group* $\mathcal{P}_{\mathcal{G}}$ of the space group $\mathcal{G}$. The point groups that can belong to space groups are called *crystallographic point groups*. □

According to Definition 1.2.5.4.1, the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is isomorphic to the point group $\mathcal{P}_{\mathcal{G}}$. This property is exploited in the graphs of *translationengleiche* subgroups of space groups, *cf.* Chapter 2.4 and Section 2.1.8.2.

All point groups in the following sections are crystallographic point groups. The maximum order of a crystallographic point group is 48 in three-dimensional space and 12 in two-dimensional space.

[8] The term *point group* is also used for a group of symmetry operations of point space, which is better called a *site-symmetry group* and which is the group describing the symmetry of the surroundings of a point in point space.

As with space groups, there are also an infinite number of crystallographic point groups which may be classified into a finite number of point-group types. This cannot be done by isomorphism because geometrically different point groups may be isomorphic. For example, point groups consisting of the identity with the inversion $\{\boldsymbol{I}, \bar{\boldsymbol{1}}\}$ or with a twofold rotation $\{\boldsymbol{I}, \boldsymbol{2}\}$ or with a reflection through a plane $\{\boldsymbol{I}, \boldsymbol{m}\}$ are all isomorphic to the (abstract) group of order 2. As for space groups, the classification may be performed, however, referring the point groups to corresponding vector bases. As translations do not occur among the point-group operations, one may choose any basis for the description of the symmetry operations by matrices. One takes the basis of $\{\boldsymbol{W}'\}$ as given and transforms the basis of $\{\boldsymbol{W}\}$ to the basis corresponding to that of $\{\boldsymbol{W}'\}$. This leads to the definition:

Definition 1.2.5.4.2. Two crystallographic point groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}'_{\mathcal{G}'}$ belong to the same *point-group type* or to the same *crystal class of point groups* if there is a real non-singular matrix $\boldsymbol{P}$ which maps a matrix group $\{\boldsymbol{W}\}$ of $\mathcal{P}_{\mathcal{G}}$ onto a matrix group $\{\boldsymbol{W}'\}$ of $\mathcal{P}'_{\mathcal{G}'}$ by the transformation $\{\boldsymbol{W}'\} = \boldsymbol{P}^{-1}\,\{\boldsymbol{W}\}\,\boldsymbol{P}$. □

Point groups can be classified by Definition 1.2.5.4.2. Further space groups may be classified into 'crystal classes of space groups' according to their point groups:

Definition 1.2.5.4.3. Two space groups belong to the same *crystal class of space groups* if their point groups belong to the same crystal class of point groups. □

Whether two space groups belong to the same crystal class or not can be worked out from their standard HM symbols: one removes the lattice parts from these symbols as well as the constituents '1' from the symbols of trigonal space groups and replaces all constituents for screw rotations and glide reflections by those for the corresponding pure rotations and reflections. The symbols obtained in this way are those of the corresponding point groups. If they agree, the space groups belong to the same crystal class. The space groups also belong to the same crystal class if the point-group symbols belong to the pair $\bar{4}2m$ and $\bar{4}m2$ or to the pair $\bar{6}2m$ and $\bar{6}m2$.

There are 32 classes of three-dimensional crystallographic point groups and 32 crystal classes of space groups, and ten classes of two-dimensional crystallographic point groups and ten crystal classes of plane groups.

The distribution into crystal classes classifies space-group types – and thus space groups – and crystallographic point groups. It does not classify the infinite set of all lattices into a finite number of lattice types, because the same lattice may belong to space groups of different crystal classes. For example, the same lattice may be that of a space group of type $P1$ (of crystal class 1) and that of a space group of type $P\bar{1}$ (of crystal class $\bar{1}$).

Nevertheless, there is also a definition of the 'point group of a lattice'. Let a vector lattice $\mathbf{L}$ of a space group $\mathcal{G}$ be referred to a lattice basis. Then the linear parts $\boldsymbol{W}$ of the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ of $\mathcal{G}$ form the point group $\mathcal{P}_{\mathcal{G}}$. If $(\boldsymbol{W}, \boldsymbol{w})$ maps the space group $\mathcal{G}$ onto itself, then the linear part $\boldsymbol{W}$ maps the (vector) lattice $\mathbf{L}$ onto itself. However, there may be additional matrices which also describe symmetry operations of the lattice $\mathbf{L}$. For example, the point group $\mathcal{P}_{\mathcal{G}}$ of a space group of type $P1$ consists of the identity $\boldsymbol{I}$ only. However, with any vector $\mathbf{t} \in \mathbf{L}$, the negative vector $-\mathbf{t} \in \mathbf{L}$ also belongs to $\mathbf{L}$. Therefore, the lattice $\mathbf{L}$ is always centrosymmetric and has the inversion $\bar{\boldsymbol{1}}$ as a symmetry operation independent of the symmetry of the space group.

Definition 1.2.5.4.4. The set of all orthogonal mappings with matrices $\boldsymbol{W}$ which map a lattice $\mathbf{L}$ onto itself is called the point group of the lattice $\mathbf{L}$ or the *holohedry* of the lattice $\mathbf{L}$. A crystal class of point groups $\mathcal{P}_{\mathcal{G}}$ is called a *holohedral crystal class* if it contains a holohedry. □

There are seven holohedral crystal classes in the space: $\bar{1}$, $2/m$, mmm, $4/mmm$, $\bar{3}m$, $6/mmm$ and $m\bar{3}m$. Their lattices are called triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal and cubic, respectively. There are four holohedral crystal classes in the plane: 2, $2mm$, $4mm$ and $6mm$. Their two-dimensional lattices (or nets) are called oblique, rectangular, square and hexagonal, respectively.

The lattices can be classified into *lattice types* or *Bravais types*, mostly called *Bravais lattices*, or into *lattice systems* (called *Bravais systems* in editions 1 to 4 of *IT* A). These classifications are not discussed here because they are not directly relevant to the classification of the space groups. This is because the lattice symmetry is not necessarily typical for the symmetry of its space group but may accidentally be higher. For example, the lattice of a monoclinic crystal may be accidentally orthorhombic (only for certain values of temperature and pressure). In Sections 8.2.5 and 8.2.7 of *IT* A the 'typical lattice symmetry' of a space group is defined.

1.2.5.5. Crystal systems and crystal families

The example of $P1$ mentioned above shows that the point group of the lattice may be systematically of higher order than that of its space group. There are obviously point groups and thus space groups that belong to a holohedral crystal class and those that do not. The latter can be assigned to a holohedral crystal class uniquely according to the following definition:[9]

Definition 1.2.5.5.1. A crystal class $\mathbf{C}$ of a space group $\mathcal{G}$ is either holohedral $\mathbf{H}$ or it can be assigned uniquely to $\mathbf{H}$ by the condition: any point group of $\mathbf{C}$ is a subgroup of a point group of $\mathbf{H}$ but not a subgroup of a holohedral crystal class $\mathbf{H}'$ of smaller order. The set of all crystal classes of space groups that are assigned to the same holohedral crystal class is called a *crystal system* of space groups. □

The 32 crystal classes of space groups are classified into seven crystal systems which are called *triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic*. There are four crystal systems of plane groups: *oblique, rectangular, square and hexagonal*. Like the space groups, the crystal classes of point groups are classified into the seven crystal systems of point groups.

Apart from accidental lattice symmetries, the space groups of different crystal systems have lattices of different symmetry. As an exception, the hexagonal primitive lattice occurs in both hexagonal and trigonal space groups as the typical lattice. Therefore, the space groups of the trigonal and the hexagonal crystal systems are more related than space groups from other different crystal systems. Indeed, in different crystallographic schools the term 'crystal system' was used for different objects. One sense of the term was the 'crystal system' as defined above, while another sense of the old term 'crystal system' is now called

[9] This assignment does hold for low dimensions of space up to dimension 4. A dimension-independent definition of the concepts of 'crystal system' and 'crystal family' is found in *IT* A, Chapter 8.2, where the classifications are treated in more detail.

a 'crystal family' according to the following definition [for definitions that are also valid in higher-dimensional spaces, see Brown *et al.* (1978) or *IT* A, Chapter 8.2]:

Definition 1.2.5.5.2. In three-dimensional space, the classification of the set of all space groups into crystal families is the same as that into crystal systems with the one exception that the trigonal and hexagonal crystal systems are united to form the *hexagonal crystal family*. There is no difference between crystal systems and crystal families in the plane. □

The partition of the space groups into crystal families is the most universal one. The space groups and their types, their crystal classes and their crystal systems are classified by the crystal families. Analogously, the crystallographic point groups and their crystal classes and crystal systems are classified by the crystal families of point groups. Lattices, their Bravais types and lattice systems can also be classified into crystal families of lattices; *cf. IT* A, Chapter 8.2.

1.2.6. Types of subgroups of space groups

1.2.6.1. Introductory remarks

Group–subgroup relations form an essential part of the applications of space-group theory. Let $\mathcal{G}$ be a space group and $\mathcal{H} < \mathcal{G}$ a proper subgroup of $\mathcal{G}$. All maximal subgroups $\mathcal{H} < \mathcal{G}$ of any space group $\mathcal{G}$ are listed in Part 2 of this volume. There are different kinds of subgroups which are defined and described in this section. The tables and graphs of this volume are arranged according to these kinds of subgroups. Moreover, for the different kinds of subgroups different data are listed in the subgroup tables and graphs.

Let $\mathcal{G}_j$ and $\mathcal{H}_j$ be space groups of the space-group types $\mathcal{G}$ and $\mathcal{H}$. The group–subgroup relation $\mathcal{G}_j > \mathcal{H}_j$ is a relation between the particular space groups $\mathcal{G}_j$ and $\mathcal{H}_j$ but it can be generalized to the space-group types $\mathcal{G}$ and $\mathcal{H}$. Certainly, not every space group of the type $\mathcal{H}$ will be a subgroup of every space group of the type $\mathcal{G}$. Nevertheless, the relation $\mathcal{G}_j > \mathcal{H}_j$ holds for any space group of $\mathcal{G}$ and $\mathcal{H}$ in the following sense: If $\mathcal{G}_j > \mathcal{H}_j$ holds for the pair $\mathcal{G}_j$ and $\mathcal{H}_j$, then for any space group $\mathcal{G}_k$ of the type $\mathcal{G}$ a space group $\mathcal{H}_k$ of the type $\mathcal{H}$ exists for which the corresponding relation $\mathcal{G}_k > \mathcal{H}_k$ holds. Conversely, for any space group $\mathcal{H}_m$ of the type $\mathcal{H}$ a space group $\mathcal{G}_m$ of the type $\mathcal{G}$ exists for which the corresponding relation $\mathcal{G}_m > \mathcal{H}_m$ holds. Only this property of the group–subgroup relations made it possible to compile and arrange the tables of this volume so that they are as concise as those of *IT* A.

1.2.6.2. Definitions and examples

'Maximal subgroups' have been introduced by Definition 1.2.4.1.2. The importance of this definition will become apparent in the corollary to Hermann's theorem, *cf.* Lemma 1.2.8.1.3. In this volume only the maximal subgroups are listed for any plane and any space group. A maximal subgroup of a plane group is a plane group, a maximal subgroup of a space group is a space group. On the other hand, a minimal supergroup of a plane group or of a space group is not necessarily a plane group or a space group, *cf.* Section 2.1.6.

If the maximal subgroups are known for each space group, then each non-maximal subgroup of a space group $\mathcal{G}$ with finite index can in principle be obtained from the data on maximal subgroups. A non-maximal subgroup $\mathcal{H} < \mathcal{G}$ of finite index $[i]$ is connected with the original group $\mathcal{G}$ through a chain $\mathcal{H} = \mathcal{Z}_k < \mathcal{Z}_{k-1} < \ldots < \mathcal{Z}_1 < \mathcal{Z}_0 = \mathcal{G}$, where each group $\mathcal{Z}_j < \mathcal{Z}_{j-1}$ is a maximal subgroup of $\mathcal{Z}_{j-1}$, with the index $[i_j] = |\mathcal{Z}_{j-1} : \mathcal{Z}_j|$, $j = 1, \ldots, k$. The number k is finite and the relation $i = \prod_{j=1}^{k} i_j$ holds, *i.e.* the total index $[i]$ is the product of the indices i_j.

According to Hermann (1929), the following types of subgroups of space groups have to be distinguished:

Definition 1.2.6.2.1. A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is called a *translationengleiche subgroup* or a *t*-subgroup of $\mathcal{G}$ if the set $\mathcal{T}(\mathcal{G})$ of translations is retained, *i.e.* $\mathcal{T}(\mathcal{H}) = \mathcal{T}(\mathcal{G})$, but the number of cosets of $\mathcal{G}/\mathcal{T}(\mathcal{G})$, *i.e.* the order P of the point group $\mathcal{P}_{\mathcal{G}}$, is reduced such that $|\mathcal{G}/\mathcal{T}(\mathcal{G})| > |\mathcal{H}/\mathcal{T}(\mathcal{H})|$.[10] □

The order of a crystallographic point group $\mathcal{P}_{\mathcal{G}}$ of the space group $\mathcal{G}$ is always finite. Therefore, the number of the subgroups of $\mathcal{P}_{\mathcal{G}}$ is also always finite and these subgroups and their relations are displayed in well known graphs, *cf.* Chapter 2.4 and Section 2.1.8 of this volume. Because of the isomorphism between the point group $\mathcal{P}_{\mathcal{G}}$ and the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, the subgroup graph for the point group $\mathcal{P}_{\mathcal{G}}$ is the same as that for the *t*-subgroups of $\mathcal{G}$, only the labels of the groups are different. For deviations between the point-group graphs and the actual space-group graphs of Chapter 2.4, *cf.* Section 2.1.8.2.

Example 1.2.6.2.2

Consider a space group $\mathcal{G}$ of type $P12/m1$ referred to a conventional coordinate system. The translation subgroup $\mathcal{T}(\mathcal{G})$ consists of all translations with translation vectors $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, where u, v, w run through all integer numbers. The coset decomposition of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ results in the four cosets $\mathcal{T}(\mathcal{G})$, $\mathcal{T}(\mathcal{G})\,\boldsymbol{2}_0$, $\mathcal{T}(\mathcal{G})\,\boldsymbol{m}_0$ and $\mathcal{T}(\mathcal{G})\,\overline{\boldsymbol{1}}_0$, where the right operations are a twofold rotation $\boldsymbol{2}_0$ around the rotation axis passing through the origin, a reflection $\boldsymbol{m}_0$ through a plane containing the origin and an inversion $\overline{\boldsymbol{1}}_0$ with the inversion point at the origin, respectively. The three combinations $\mathcal{H}_1 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\,\boldsymbol{2}_0$, $\mathcal{H}_2 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\,\boldsymbol{m}_0$ and $\mathcal{H}_3 = \mathcal{T}(\mathcal{G}) \cup (\mathcal{T}\mathcal{G})\,\overline{\boldsymbol{1}}_0$ each form a *translationengleiche* maximal subgroup of $\mathcal{G}$ of index 2 with the space-group symbols $P121$, $P1m1$ and $P\overline{1}$, respectively.

Definition 1.2.6.2.3. A subgroup $\mathcal{H} < \mathcal{G}$ of a space group $\mathcal{G}$ is called a *klassengleiche subgroup* or a *k-subgroup* if the set $\mathcal{T}(\mathcal{G})$ of all translations of $\mathcal{G}$ is reduced to $\mathcal{T}(\mathcal{H}) < \mathcal{T}(\mathcal{G})$ but all linear parts of $\mathcal{G}$ are retained. Then the number of cosets of the decompositions $\mathcal{H}/\mathcal{T}(\mathcal{H})$ and $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is the same, *i.e.* $|\mathcal{H}/\mathcal{T}(\mathcal{H})| = |\mathcal{G}/\mathcal{T}(\mathcal{G})|$. In other words: the order of the point group $\mathcal{P}_{\mathcal{H}}$ is the same as that of $\mathcal{P}_{\mathcal{G}}$. See also footnote 10. □

For a *klassengleiche* subgroup $\mathcal{H} < \mathcal{G}$, the cosets of the factor group $\mathcal{H}/\mathcal{T}(\mathcal{H})$ are smaller than those of $\mathcal{G}/\mathcal{T}(\mathcal{G})$. Because $\mathcal{T}(\mathcal{H})$ is still infinite, the number of elements of each coset is infinite but the index $|\mathcal{T}(\mathcal{G}) : \mathcal{T}(\mathcal{H})| > 1$ is finite. The number of *k*-subgroups of $\mathcal{G}$ is always infinite.

[10] German: *zellengleiche* means 'with the same cell'; *translationengleiche* means 'with the same translations'; *klassengleiche* means 'of the same (crystal) class'. Of the different German declension endings only the form with terminal *-e* is used in this volume. The terms *zellengleiche* and *klassengleiche* were introduced by Hermann (1929). The term *zellengleiche* was later replaced by *translationengleiche* because of possible misinterpretations. In this volume they are sometimes abbreviated as *t*-subgroups and *k*-subgroups.

references