International Tables for Crystallography (2011). Vol. A1, Section 1.2.5.3, pp. 15–16.

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 'superclass'. 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.