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8.2. Classifications of space groups, point groups and lattices

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8.2.1. Introduction

One of the main tasks of theoretical crystallography is to sort the infinite number of conceivable crystal patterns into a finite number of classes, where the members of each class have certain properties in common. In such a classification, each crystal pattern is assigned only to one class. The elements of a class are called equivalent, the classes being equivalence classes in the mathematical sense of the word. Sometimes the word 'type' is used instead of 'class'.

An important principle in the classification of crystals and crystal patterns is symmetry, in particular the space group of a crystal pattern. The different classifications of space groups discussed here are displayed in Fig. 8.2.1.1.

Classification of crystals according to symmetry implies three steps. First, criteria for the symmetry classes have to be defined. The second step consists of the derivation and complete listing of the possible symmetry classes. The third step is the actual assignment of the existing crystals to these symmetry classes. In this chapter, only the first step is dealt with. The space-group tables of this volume are the result of the second step. The third step is beyond the scope of this volume.

8.2.2. Space-group types

The finest commonly used classification of three-dimensional space groups, *i.e.* the one resulting in the highest number of classes, is the *classification into the* 230 *(crystallographic) space-group types.** The word 'type' is preferred here to the word 'class', since in crystallography 'class' is already used in the sense of 'crystal class', *cf.* Sections 8.2.3 and 8.2.4. The classification of space groups into space-group types reveals the common symmetry properties of all space groups belonging to one type. Such common properties of the space groups can be considered as 'properties of the space-group types'.

The practising crystallographer usually assumes the 230 space-group types to be known and to be described in this volume by representative data such as figures and tables. To the experimentally determined space group of a particular crystal structure, *e.g.* of pyrite FeS_2, the corresponding space-group type No. 205 ($Pa\bar{3} \equiv T_h^6$) of *International Tables* is assigned. Two space groups, *e.g.* those of FeS_2 and CO_2, belong to the same space-group type if their symmetries correspond to the same entry in *International Tables.*

The rigorous definition of the classification of space groups into space-group types can be given in a more geometric or a more algebraic way. Here matrix algebra will be followed, by which primarily the classification into the 219 so-called *affine space-group types* is obtained.† For this classification, each space group is referred to a primitive basis and an origin. In this case, the matrices $\boldsymbol{W}_j$ of the symmetry operations consist of integral coefficients and $\det(\boldsymbol{W}_j) = \pm 1$ holds. Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are then represented by their $(n+1) \times (n+1)$ matrix groups $\{\mathbb{W}\}$ and $\{\mathbb{W}'\}$. These two matrix groups are now compared.

Definition: The space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same *space-group type* if, for each primitive basis and each origin of $\mathcal{G}$, a primitive basis and an origin of $\mathcal{G}'$ can be found so that the matrix groups $\{\mathbb{W}\}$ and $\{\mathbb{W}'\}$ are identical. In terms of matrices, this can be expressed by the following definition:

Definition: The space groups $\mathcal{G}$ and $\mathcal{G}'$ *belong to the same space-group type* if an $(n+1) \times (n+1)$ matrix $\mathbb{P}$ exists, for which the matrix part $\boldsymbol{P}$ is an integral matrix with $\det(\boldsymbol{P}) = \pm 1$ and the column part $\boldsymbol{p}$ consists of real numbers, such that

$$\{\mathbb{W}'\} = \mathbb{P}^{-1}\{\mathbb{W}\}\mathbb{P} \qquad (8.2.2.1)$$

holds. The matrix part $\boldsymbol{P}$ of $\mathbb{P}$ describes the transition from the primitive basis of $\mathcal{G}$ to the primitive basis of $\mathcal{G}'$. The column part $\boldsymbol{p}$ of $\mathbb{P}$ expresses the (possibly) different origin choices for the descriptions of $\mathcal{G}$ and $\mathcal{G}'$.

Equation (8.2.2.1) is an equivalence relation for space groups. The corresponding classes are called *affine space-group types*. By this definition, one obtains 17 plane-group types for E^2 and 219 space-group types for E^3, see Fig. 8.2.1.1. Listed in the space-group

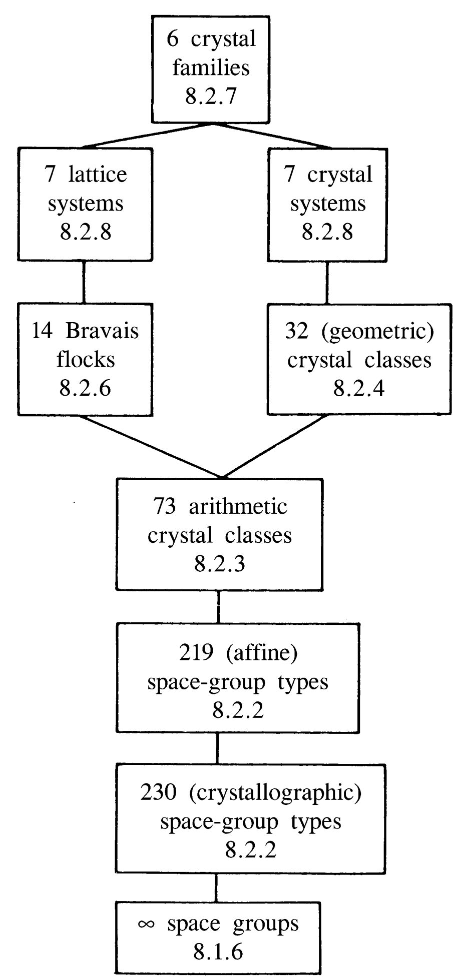

Fig. 8.2.1.1. Classifications of space groups. In each box, the number of classes, *e.g.* 32, and the section in which the corresponding term is defined, *e.g.* 8.2.4, are stated.

* These space-group types are often denoted by the word 'space group' when speaking of the 17 'plane groups' or of the 219 or 230 'space groups'. In a number of cases, the use of the same word 'space group' with two different meanings ('space group' and 'space-group type' which is an infinite set of space groups) is of no further consequence. In some cases, however, it obscures important relations. For example, it is impossible to appreciate the concept of isomorphic subgroups of a space group if one does not strictly distinguish between space groups and space-group types: *cf.* Section 8.3.3 and Part 13.

† According to the 'Theorem of Bieberbach', in all dimensions the classification into affine space-group types results in the same types as the classification into *isomorphism types of space groups*. Thus, the affine equivalence of different space groups can also be recognized by purely group-theoretical means: *cf.* Ascher & Janner (1965, 1968/69).

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tables are 17 plane-group types for E^2 and 230 space-group types for E^3. Obviously, the equivalence definition of the space-group tables differs somewhat from the one used above. In practical crystallography, one wants to distinguish between right- and left-handed screws and does not want to change from a right-handed to a left-handed coordinate system. In order to avoid such transformations, the matrix $\boldsymbol{P}$ of equation (8.2.2.1) is restricted by the additional condition $\det(\boldsymbol{P}) = +1$. Using matrices $\mathbb{P}$ with $\det(\boldsymbol{P}) = +1$ only, 11 space-group types of E^3 split into pairs, which are the so-called pairs of *enantiomorphic space-group types*. The Hermann–Mauguin and Schoenflies symbols (in parentheses) of the pairs of enantiomorphic space-group types are $P4_1$–$P4_3$ (C_4^2–C_4^4), $P4_122$–$P4_322$ (D_4^3–D_4^7), $P4_12_12$–$P4_32_12$ (D_4^4–D_4^8), $P3_1$–$P3_2$ (C_3^2–C_3^3), $P3_121$–$P3_221$ (D_3^4–D_3^6), $P3_112$–$P3_212$ (D_3^3–D_3^5), $P6_1$–$P6_5$ (C_6^2–C_6^3), $P6_2$–$P6_4$ (C_6^4–C_6^5), $P6_122$–$P6_522$ (D_6^2–D_6^3), $P6_222$–$P6_422$ (D_6^4–D_6^5) and $P4_132$–$P4_332$ (O^7–O^6). In order to distinguish between the two definitions of space-group types, the first is called the classification into the 219 *affine space-group types* and the second the classification into the 230 *crystallographic* or *positive affine* or *proper affine space-group types*, see Fig. 8.2.1.1. Both classifications are useful.

In Section 8.1.6, symmorphic space groups were defined. It can be shown (with either definition of space-group type) that all space groups of a space-group type are symmorphic if one of these space groups is symmorphic. Therefore, it is also possible to speak of types of symmorphic and non-symmorphic space groups. In E^3, symmorphic space groups do not occur in enantiomorphic pairs. This does happen, however, in E^4.

The so-called space-group symbols are really symbols of 'crystallographic space-group types'. There are several different kinds of symbols (for details see Part 12). The *numbers* denoting the crystallographic space-group types and the *Schoenflies symbols* are unambiguous but contain little information. The *Hermann–Mauguin symbols* depend on the choice of the coordinate system but they are much more informative than the other notations.

8.2.3. Arithmetic crystal classes

As space groups not only of the same type but also of different types have symmetry properties in common, coarser classifications can be devised which are classifications of both space-group types and individual space groups. The following classifications are of this kind. Again each space group is referred to a *primitive* basis and an origin.

Definition: All those space groups belong to the same *arithmetic crystal class* for which the matrix parts are identical if suitable primitive bases are chosen, irrespective of their column parts.

Algebraically, this definition may be expressed as follows. Equation (8.2.2.1) of Section 8.2.2 relating space groups of the same type may be written more explicitly as follows:

$$\{(\boldsymbol{W}', \boldsymbol{w}')\} = \{[\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}, \boldsymbol{P}^{-1}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p})]\}, \qquad (8.2.3.1)$$

the matrix part of which is

$$\{\boldsymbol{W}'\} = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\}. \qquad (8.2.3.2)$$

Space groups of different types belong to the same arithmetic crystal class if equation (8.2.3.2), but not equation (8.2.2.1) or equation (8.2.3.1), is fulfilled, *e.g.* space groups of types $P2$ and $P2_1$. This gives rise to the following definition:

Definition: Two space groups belong to the same *arithmetic crystal class* of space groups if there is an *integral* matrix $\boldsymbol{P}$ with $\det(\boldsymbol{P}) = \pm 1$ such that

$$\{\boldsymbol{W}'\} = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\} \qquad (8.2.3.2)$$

holds.

By definition, both space groups and space-group types may be classified into arithmetic crystal classes. It is apparent from equation (8.2.3.2) that 'arithmetic equivalence' refers only to the matrix parts and not to the column parts of the symmetry operations. Among the space-group types of each arithmetic crystal class there is exactly one for which the column parts vanish for a suitable choice of the origin. This is the symmorphic space-group type, *cf.* Sections 8.1.6 and 8.2.2. The nomenclature for arithmetic crystal classes makes use of this relation: The lattice letter and the point-group part of the Hermann–Mauguin symbol for the symmorphic space-group type are interchanged to designate the arithmetic crystal class, *cf.* de Wolff *et al.* (1985). This symbolism enables one to recognize easily the arithmetic crystal class to which a space group belongs: One replaces in the Hermann–Mauguin symbol of the space group all screw rotations and glide reflections by the corresponding rotations and reflections and interchanges then the lattice letter and the point-group part.

Examples

The space groups with Hermann–Mauguin symbols $P2/m$, $P2_1/m$, $P2/c$ and $P2_1/c$ belong to the arithmetic crystal class $2/mP$, whereas $C2/m$ and $C2/c$ belong to the different arithmetic crystal class $2/mC$. The space groups with symbols $P31m$ and $P31c$ form the arithmetic crystal class $31mP$; those with symbols $P3m1$ and $P3c1$ form the different arithmetic crystal class $3m1P$. A further arithmetic crystal class, $3mR$, is composed of the space groups $R3m$ and $R3c$.

Remark: In order to belong to the same arithmetic crystal class, space groups must belong to the same geometric crystal class, *cf.* Section 8.2.4 and to the same Bravais flock; *cf.* Section 8.2.6. These two conditions, however, are only necessary but not sufficient.

There are 13 arithmetic crystal classes of plane groups in E^2 and 73 arithmetic crystal classes of space groups in E^3, see Fig. 8.2.1.1. Arithmetic crystal classes are rarely used in practical crystallography, even though they play some role in structural crystallography because the 'permissible origins' (see Giacovazzo, 2002) are the same for all space groups of one arithmetic crystal class. The classification of space-group types into arithmetic crystal classes, however, is of great algebraic consequence. In fact, the arithmetic crystal classes are the basis for the further classifications of space groups.

In E^3, enantiomorphic pairs of space groups always belong to the same arithmetic crystal class. Enantiomorphism of arithmetic crystal classes can be defined analogously to enantiomorphism of space groups. It does not occur in E^2 and E^3, but appears in spaces of higher dimensions, *e.g.* in E^4; *cf.* Brown *et al.* (1978).

In addition to space groups, equation (8.2.3.2) also classifies the set of all finite integral-matrix groups. Thus, one can speak of *arithmetic crystal classes of finite integral-matrix groups.* It is remarkable, however, that this classification of the matrix groups does *not* imply a classification of the corresponding point groups. Although *every* finite integral-matrix group represents the point group of some space group, referred to a primitive coordinate basis, there are *no* arithmetic crystal classes of point groups. For example, space-group types $P2$ and $C2$ both have point groups of the same type, 2, but referred to primitive bases their (3×3) matrix groups are not arithmetically equivalent, *i.e.* there is no integral matrix $\boldsymbol{P}$ with $\det(\boldsymbol{P}) = \pm 1$, such that equation (8.2.3.2) holds.

The arithmetic crystal classes of finite integral-matrix groups are the basis for the classification of lattices into Bravais types of

references