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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

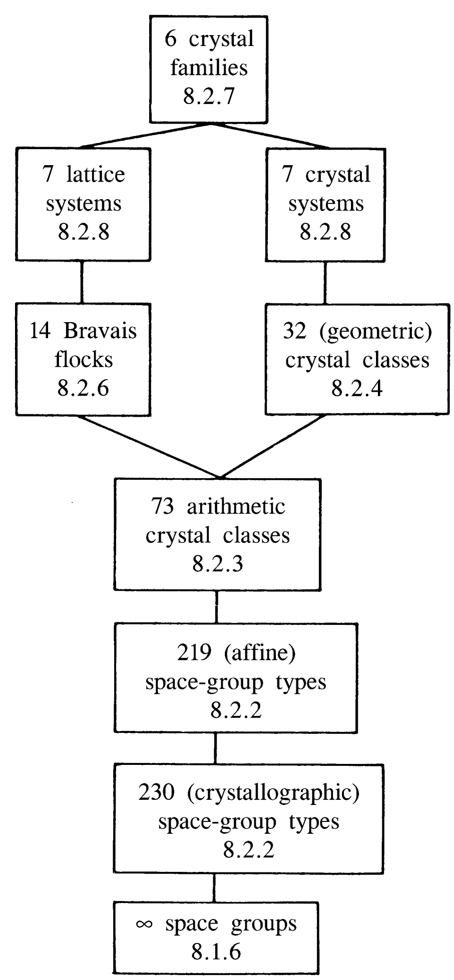

Fig. 8.2.1.1. Classifications of space groups. In each box, the number of classes, *e.g.* 32, and the section in which the corresponding term is defined, *e.g.* 8.2.4, are stated.

* 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).

references