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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

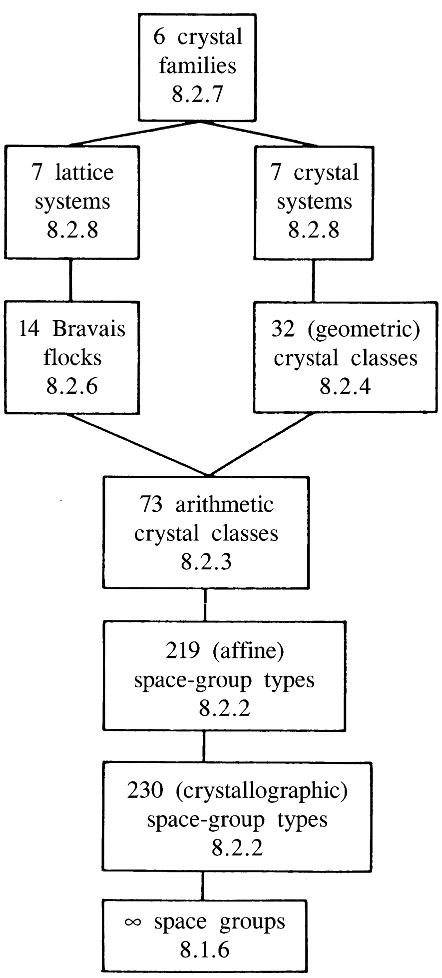

Fig. 8.2.1.1. Classifications of space groups. In each box, the number of classes, *e.g.* 32, and the section in which the corresponding term is defined, *e.g.* 8.2.4, are stated.

* 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).

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 lattices: see Section 8.2.5. Even though the consideration of finite integral-matrix groups in connection with space groups is not common in practical crystallography, these matrix groups play a very important role in the classifications discussed in subsequent sections. Finite integral-matrix groups have the advantage of being particularly suitable for computer calculations.

8.2.4. Geometric crystal classes

The widely used term 'crystal class' corresponds to the 'geometric crystal class' described in this section, and must be distinguished from the 'arithmetic' crystal class, introduced in Section 8.2.3. Geometric crystal classes classify the space groups *and* their point groups, *i.e.* the symmetry groups of the external shape of macroscopic crystals. Classification by morphological symmetry was done long before space groups were known. In Section 8.1.6, the reasons are stated why the two seemingly different classifications agree, namely that of space groups according to their matrix groups $\{\boldsymbol{W}\}$, and that of macroscopic crystals according to the 'point groups' of their sets of face normals.

To define geometric crystal classes, we again compare the matrix parts of the space groups.

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

In contrast to the definition of arithmetic crystal classes, nonprimitive bases are admitted. To express this definition in matrix terms, we refer to equation (8.2.3.2) of the previous section.

Definition: Two space groups belong to the same *geometric crystal class* or *crystal class* if there is a *real* matrix $\boldsymbol{P}$ such that

$$\{\boldsymbol{W}'\} = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\} \qquad (8.2.4.1)$$

holds.

In contrast to arithmetic crystal classes where $\boldsymbol{P}$ is a *unimodular integral* matrix, for geometric crystal classes only a *real* matrix $\boldsymbol{P}$ is required. Thus, the restriction $\det(\boldsymbol{P}) = \pm 1$ is no longer necessary, $\det(\boldsymbol{P})$ may have any value except zero.

Example

Referred to appropriate primitive bases, the matrix parts of mirror and glide reflections in space groups *Pm* and *Cm* are

$$\boldsymbol{W}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \boldsymbol{W}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

respectively. There is no integral matrix $\boldsymbol{P}$ with $\det(\boldsymbol{P}) = \pm 1$ for which equation (8.2.3.2) holds because $\det(\boldsymbol{P}) = 2(P_{11}P_{22}P_{33} - P_{31}P_{22}P_{13})$.

Thus, *Pm* and *Cm* are members of different arithmetic crystal classes. The matrix

$$\boldsymbol{P} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ with } \det(\boldsymbol{P}) = 2,$$

however, does solve equation (8.2.4.1) and, therefore, *Pm* and *Cm* are members of the same geometric crystal class, as are *Pc* and *Cc*.

Clearly, space groups of the same arithmetic crystal class always obey condition (8.2.4.1). Thus, the geometric crystal classes form a classification not only of space groups and space-group types but also of arithmetic crystal classes. There are ten geometric crystal classes in E^2 and 32 geometric crystal classes in E^3; see Fig. 8.2.1.1. As $\{(\boldsymbol{W})\}$ is a matrix representation of the point group of a space group, the definition may be restated as follows:

Definition: Two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same geometric crystal class if the matrix representations $\{\boldsymbol{W}\}$ and $\{\boldsymbol{W}'\}$ of their point groups are equivalent, *i.e.* if there is a real matrix $\boldsymbol{P}$ such that equation (8.2.4.1) holds.

This definition may also be used to classify point groups, *via* their matrix groups, into *geometric crystal classes of point groups*. Moreover, the geometric crystal classes provide a classification of the finite groups of integral matrices. Again, matrix groups of the same arithmetic crystal class always belong to the same geometric crystal class.

Enantiomorphism of geometric crystal classes may occur in dimensions greater than three, as it does for arithmetic crystal classes.

8.2.5. Bravais classes of matrices and Bravais types of lattices (*lattice types*)

Every space group $\mathcal{G}$ has a vector lattice **L** of translation vectors. The elements of the point group $\mathcal{P}$ of $\mathcal{G}$ are symmetry operations of **L**. The lattice **L** of $\mathcal{G}$, however, may have additional symmetry in comparison with $\mathcal{P}$.

The symmetry of a vector lattice **L** is its point group according to the following definition:

Definition: The group $\mathcal{D}$ of *all* linear mappings which map a vector lattice **L** onto itself is called the *point group* or the *point symmetry of the lattice* **L**. Those geometric crystal classes to which point symmetries of lattices belong are called *holohedries*.

The inversion $\mathbf{x} \rightarrow -\mathbf{x}$ is always a symmetry operation of **L**, even if $\mathcal{G}$ does not contain inversions. If, for instance, $\mathcal{G}$ belongs to space-group type $P6_3mc$, its point group $\mathcal{P}$ is 6*mm* but the point symmetry $\mathcal{D}$ of **L** is $6/mmm$. Thus, the point group $\mathcal{D}$ of the lattice **L** is of higher order than the point group $\mathcal{P}$ of $\mathcal{G}$.

Other symmetry operations of **L** may also have no counterpart in $\mathcal{G}$. Space groups of type $P6_3/m$, for instance, have inversions but no reflections across 'vertical' mirror planes. The point symmetry of their lattices again is $6/mmm$, *i.e.* in this case too there are more elements in the point group $\mathcal{D}$ of **L** than in the point group $\mathcal{P}$ of $\mathcal{G}$.

For purposes of classification, lattices **L** will now be considered independently of their space groups $\mathcal{G}$. Associated with each vector lattice **L** is a finite group $\mathcal{L}$ of $(n \times n)$ integral matrices which describes the point group $\mathcal{D}$ of **L** with respect to some primitive basis of **L**. This matrix group $\mathcal{L}$ is a member of an arithmetic crystal class; *cf.* Section 8.2.3. Thus, there are some arithmetic crystal classes with matrix groups $\mathcal{L}$ of lattices, *e.g.* the arithmetic crystal class $6/mmmP$. Other arithmetic crystal classes, however, are not associated with lattices, like $6/mP$ or 6*mmP*. One can distinguish these two cases with the following definition:

Definition: An arithmetic crystal class with matrix groups $\mathcal{L}$ of lattices is called a Bravais arithmetic crystal class or a *Bravais class*.

By this definition, each lattice is associated with a Bravais class. On the other hand, each matrix group of a Bravais class represents the point group of a lattice referred to an appropriate primitive basis. Closer inspection shows that there are five Bravais classes of E^2 and 14 of E^3. With the use of Bravais classes, lattices may be classified using the following definition:

Definition: All those vector lattices belong to the same *Bravais type or lattice type of vector lattices*, for which the matrix groups belong to the same Bravais class.

Thus, five Bravais types of lattices exist in E^2, and 14 in E^3. This classification can be transferred from vector lattices **L** to point lattices *L*. To each point lattice *L* a vector lattice **L** is uniquely assigned. Thus, one can define Bravais types of point lattices *via* the Bravais types of vector lattices by the definition:

Definition: All those point lattices belong to the same *Bravais type of point lattices* for which the vector lattices belong to the same Bravais type of (vector) lattices.

Usually the Bravais types are called 'the five' or 'the 14 Bravais lattices' of E^2 or E^3. It must be emphasized, however, that 'Bravais lattices' are not individual lattices but types (or classes) of all lattices with certain common properties. Geometrically, these common properties are expressed by the 'centring type' and the well known relations between the lattice parameters, provided the lattices are referred to conventional bases, *cf.* Chapters 2.1 and 9.1. In these chapters a nomenclature of Bravais types is presented.

8.2.6. Bravais flocks of space groups

Another plausible classification of space groups and space-group types, as well as of arithmetic crystal classes, is based on the lattice of the space group. One is tempted to use the definition: 'Two space groups are members of the same class if their lattices belong to the same Bravais type'. There is, however, a difficulty which will become apparent by an example.

It was shown in Section 8.2.5 with the two examples of space groups $P6_3mc$ and $P6_3/m$ that the lattice **L** of the space group $\mathcal{G}$ may *systematically* have higher symmetry than the point group $\mathcal{P}$ of $\mathcal{G}$. The lattice **L**, however, may also *accidentally* have higher symmetry than $\mathcal{P}$ because the lattice parameters may have special metrical values.

Example

For a monoclinic crystal structure at some temperature T_1, the monoclinic angle β may be equal to 91°, whereas, for the same monoclinic crystal structure at some other temperature T_2, $\beta = 90°$ may hold. In this case, the lattice **L** at temperature T_2, if considered to be detached from the crystal structure and its space group, has orthorhombic symmetry, because all the symmetry operations of an orthorhombic lattice map **L** onto itself. The lattice **L** at other temperatures, however, has always monoclinic symmetry.

This is of importance for the practising crystallographer, because quite often difficulties arise in the interpretation of X-ray powder diagrams if no single crystals are available. In some cases, changes of temperature or pressure may enable one to determine the true symmetry of the substance. The example shows, however, that the lattices of different space groups of the same space-group type *may* have different symmetries. The possibility of accidental lattice symmetry prevents the direct use of lattice types for a rigorous classification of space-group types.

Such a classification is possible, however, *via* the point group $\mathcal{P}$ of the space group $\mathcal{G}$ and its matrix groups. Referred to a primitive basis, the point group $\mathcal{P}$ of $\mathcal{G}$ is represented by a finite group of integral $(n \times n)$ matrices which belongs to some arithmetic crystal class. This matrix group can be uniquely assigned to a Bravais class: It either belongs already to a Bravais class, *e.g.* for space groups *Pmna* and $C2/c$, or it may be uniquely connected to a Bravais class by the following two conditions:

(i) The matrix group of $\mathcal{P}$ is a subgroup of a matrix group of the Bravais class.

(ii) The order of the matrix group of the Bravais class is the smallest possible one compatible with condition (i).

Example

A space group of type $I4_1$ belongs to the arithmetic crystal class 4*I*. The Bravais classes fulfilling condition (i) are $4/mmmI$ and $m\bar{3}mI$. With condition (ii), the Bravais class $m\bar{3}mI$ is excluded. Thus, the space group $I4_1$ is uniquely assigned to the Bravais class $4/mmmI$. Even though, with accidental lattice parameters $a = b = c = 5$ Å, the symmetry of the lattice alone is higher, namely $Im\bar{3}m$, this does not change the Bravais class of $I4_1$.

This assignment leads to the definition:

Definition: Space groups that are assigned to the same Bravais class belong to the same *Bravais flock of space groups.*

By this definition, the space group $I4_1$ mentioned above belongs to the Bravais flock of $4/mmmI$, despite the fact that the Bravais class of the lattice may be $m\bar{3}mI$ as a result of accidental symmetry.

Obviously, to each Bravais class a Bravais flock corresponds. Thus, there exist five Bravais flocks of plane groups and 14 Bravais flocks of space groups, see Fig. 8.2.1.1, and the Bravais flocks may be denoted by the symbols of the corresponding Bravais classes; *cf.* Section 8.2.5.

Though Bravais flocks themselves are of little practical importance, they are necessary for the definition of crystal families and lattice systems, as described in Sections 8.2.7 and 8.2.8.

8.2.7. Crystal families

Another classification of space groups, which is a classification of geometric crystal classes and Bravais flocks as well, is that into crystal families.

Definition: A *crystal family** is the smallest set of space groups containing, for any of its members, all space groups of the Bravais flock and all space groups of the geometric crystal class to which this member belongs.

Example

The space-group types *R*3 and $P6_1$ belong to the same crystal family because both *R*3 and *P*3 belong to the geometric crystal class 3, whereas both *P*3 and $P6_1$ are members of the same Bravais flock $6/mmmP$. In this example, *P*3 serves as a link between *R*3 and $P6_1$.

There are four crystal families in E^2 (oblique *m*, rectangular *o*, square *t* and hexagonal *h*) and six crystal families in E^3 [triclinic (anorthic) *a*, monoclinic *m*, orthorhombic *o*, tetragonal *t*, hexagonal *h* and cubic *c*]; see Fig. 8.2.1.1.

The classification into crystal families is a rather universal crystallographic concept as it applies to many crystallographic objects: space groups, space-group types, arithmetic and geometric crystal classes of space groups, point groups (morphology of crystals), lattices and Bravais types of lattices.

Remark: In most cases of E^2 and E^3, the lattices of a given crystal family of lattices have the same point symmetry (for the symbols, see Table 2.1.2.1): rectangular *op* and *oc* in E^2; monoclinic *mP* and *mS*, orthorhombic *oP*, *oS*, *oF* and *oI*, tetragonal *tP* and *tI*, cubic *cP*, *cF* and *cI* in E^3. Only to the hexagonal crystal family in E^3 do lattices with two different point symmetries belong: the hexagonal lattice type *hP* with point symmetry $6/mmm$ and the rhombohedral

* The classes defined here have been called 'crystal families' by Neubüser *et al.* (1971). For the same concept the term 'crystal system' has been used, particularly in American and Russian textbooks. In these *Tables,* however, 'crystal system' designates a different classification, described in Section 8.2.8. To avoid confusion, the term 'crystal family' is used here.

Table 8.2.8.1. *Distribution of trigonal and hexagonal space groups into crystal systems and lattice systems*

The hexagonal lattice system is also the hexagonal Bravais flock, the rhombohedral lattice system is the rhombohedral Bravais flock.

		Hexagonal lattice system	Rhombohedral lattice system
Crystal system	Crystal class	Hexagonal Bravais flock	Rhombohedral Bravais flock
Hexagonal	$6/mmm$	$P6/mmm$, $P6/mcc$, $P6_3/mcm$, $P6_3/mmc$	
	$\bar{6}2m$	$P\bar{6}m2$, $P\bar{6}c2$, $P\bar{6}2m$, $P\bar{6}2c$	
	$6mm$	$P6mm$, $P6cc$, $P6_3cm$, $P6_3mc$	
	622	$P622$, $P6_122$, ..., $P6_322$	
	$6/m$	$P6/m$, $P6_3/m$	
	$\bar{6}$	$P\bar{6}$	
	6	$P6$, $P6_1$, $P6_5$, $P6_2$, $P6_4$, $P6_3$	
Trigonal	$\bar{3}m$	$P\bar{3}1m$, $P\bar{3}1c$, $P\bar{3}m1$, $P\bar{3}c1$	$R\bar{3}m$, $R\bar{3}c$
	$3m$	$P3m1$, $P31m$, $P3c1$, $P31c$	$R3m$, $R3c$
	32	$P312$, $P321$, $P3_112$, $P3_121$, $P3_212$, $P3_221$	$R32$
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$
	3	$P3$, $P3_1$, $P3_2$	$R3$

lattice type *hR* with point symmetry $\bar{3}m$. In E^4 and higher dimensions, such cases are much more abundant.

Usually, the same type of coordinate system, the so-called 'conventional coordinate system', is used for all space groups of a crystal family, for instance 'hexagonal axes' for both hexagonal and rhombohedral lattices; *cf.* Chapters 2.1, 2.2 and 9.1. Other coordinate systems, however, may be used when convenient. To avoid confusion, the use of unconventional coordinate systems should be stated explicitly.

8.2.8. Crystal systems and lattice systems*

At least three different classifications of space groups, crystallographic point groups and lattice types have been called 'crystal systems' in crystallographic literature. Only one of them classifies space groups, crystallographic point groups *and* lattice types. It has been introduced in the preceding section under the name 'crystal families'. The two remaining classifications are called here 'crystal systems' and 'lattice systems', and are considered in this section. Crystal systems classify space groups and crystallographic point groups but *not* lattice types. Lattice systems classify space groups and lattice types but *not* crystallographic point groups.

The '*crystal-class systems*' or '*crystal systems*' are used in these *Tables.* In E^2 and E^3, the crystal systems provide the same classification as the crystal families, with the exception of the hexagonal crystal family in E^3. Here, the hexagonal family is subdivided into the *trigonal* and the *hexagonal* crystal system. Each of these crystal systems consists of complete geometric crystal classes of space groups. The space groups of the five trigonal crystal classes 3, $\bar{3}$, 32, $3m$ and $\bar{3}m$ belong to either the hexagonal or the rhombohedral Bravais flock, and both Bravais flocks are represented in each of these crystal classes. The space groups of the seven hexagonal crystal classes 6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}2m$ and $6/mmm$, however, belong only to the hexagonal Bravais flock.

These observations will be used to define crystal systems by the concept of intersection. A geometric crystal class and a Bravais flock of space groups are said to *intersect* if there is at least one space group common to both. Accordingly, the rhombohedral Bravais flock intersects all trigonal crystal classes but none of the hexagonal crystal classes. The hexagonal Bravais flock, on the other hand, intersects all trigonal *and* hexagonal crystal classes, see Table 8.2.8.1.

Using the concept of intersection, one obtains the definition:

Definition: A crystal-class system or a *crystal system* contains complete geometric crystal classes of space groups. All those geometric crystal classes belong to the same crystal system which intersect exactly the same set of Bravais flocks.

There are four crystal systems in E^2 and seven in E^3. The classification into crystal systems applies to space groups, space-group types, arithmetic crystal classes and geometric crystal classes, see Fig. 8.2.1.1. Moreover, *via* their geometric crystal classes, the crystallographic point groups are classified by 'crystal systems of point groups'. Historically, point groups were the first to be classified by crystal systems. Bravais flocks of space groups and Bravais types of lattices are not classified, as members of both can occur in more than one crystal system. For example, $P3$ and $P6_1$ belong to the same hexagonal Bravais flock but to different crystal systems, $P3$ to the trigonal, $P6_1$ to the hexagonal crystal system. Thus, a crystal system of space groups does not necessarily contain complete Bravais flocks (it does so, however, in E^2 and in all crystal systems of E^3, except for the trigonal and hexagonal systems).

The use of crystal systems has some practical advantages.

(i) Classical crystal physics considers physical properties of anisotropic continua. The symmetry of these properties as well as the symmetry of the external shape of a crystal are determined by point groups. Thus, crystal systems provide a classification for both tensor properties and morphology of crystals.

(ii) The 11 'Laue classes' determine both the symmetry of X-ray photographs (if Friedel's rule is valid) and the symmetry of the physical properties that are described by polar tensors of even rank and axial tensors of odd rank. Crystal systems classify Laue classes.

(iii) The correspondence between trigonal, tetragonal and hexagonal crystal classes becomes visible, as displayed in Table 10.1.1.2.

Whereas crystal systems classify geometric crystal classes and point groups, lattice systems classify Bravais flocks and Bravais types of lattices. Lattice systems may be defined in two ways. The first definition is analogous to that of crystal systems and uses once again the concept of intersection, introduced above.

Definition: A *lattice system* of space groups contains complete Bravais flocks. All those Bravais flocks which intersect exactly the same set of geometric crystal classes belong to the same lattice system, *cf.* footnote to heading of this section.

There are four lattice systems in E^2 and seven lattice systems in E^3. In E^2 and E^3, the classification into lattice systems is the same as that into crystal families and crystal systems except for the hexagonal crystal family of E^3. The space groups of the hexagonal Bravais flock (lattice letter *P*) belong to the twelve geometric crystal classes from 3 to $6/mmm$, whereas the space groups of the rhombohedral Bravais flock (lattice letter *R*) only belong to the five geometric crystal classes 3, $\bar{3}$, 32, $3m$ and $\bar{3}m$. Thus, these two Bravais flocks form the hexagonal and the rhombohedral lattice systems with 45 and 7 types of space groups, respectively.

The lattice systems provide a classification of space groups, see Fig. 8.2.1.1. Geometric crystal classes are not classified, as they can

* 'Lattice systems' were called 'Bravais systems' in editions 1 to 4 of this volume. The name has been changed because in practice 'Bravais systems' may be confused with 'Bravais types' or 'Bravais lattices'.

occur in more than one lattice system. For example, space groups $P3_1$ and $R3$, both of crystal class 3, belong to the hexagonal and rhombohedral lattice systems, respectively.

The above definition of lattice systems corresponds closely to the definition of crystal systems. There exists, however, another definition of lattice systems which emphasizes the geometric aspect more. For this it should be remembered that each Bravais flock is related to the point symmetry of a lattice type *via* its Bravais class; *cf.* Sections 8.2.5 and 8.2.6. It can be shown that Bravais flocks intersect the same set of crystal classes if their Bravais classes belong to the same (holohedral) geometric crystal class. Therefore, one can use the definition:

Definition: A *lattice system* of space groups contains complete Bravais flocks. All those Bravais flocks belong to the same lattice system for which the Bravais classes belong to the same (holohedral) geometric crystal class.

According to this second definition, it is sufficient to compare only the Bravais classes instead of all space groups of different Bravais flocks. The comparison of Bravais classes can be replaced by the comparison of their holohedries; *cf.* Section 8.2.5. This gives rise to a special advantage of lattice systems, the possibility of classifying lattices and lattice types. (Such a classification is not possible using crystal systems.) All those lattices belong to the same *lattice system of lattices* for which the lattice point groups belong to the same holohedry. As lattices of the same lattice type always belong to the same holohedry, lattice systems also classify lattice types.

The adherence of a space group of the hexagonal crystal family to the trigonal or hexagonal crystal system and the rhombohedral or hexagonal lattice system is easily recognized by means of its Hermann–Mauguin symbol. The Hermann–Mauguin symbols of the trigonal crystal system display a '3' or '$\bar{3}$', those of the hexagonal crystal system a '6' or '$\bar{6}$'. On the other hand, the rhombohedral lattice system displays lattice letter '*R*' and the hexagonal one '*P*' in the Hermann–Mauguin symbols of their space groups.

It should be mentioned that the lattice system of the lattice of a space group may be different from the lattice system of the space group itself. This always happens if the lattice symmetry is accidentally higher than is required by the space group, *e.g.* for a monoclinic space group with an orthorhombic lattice, *i.e.* $\beta = 90°$, or a tetragonal space group with cubic metrics, *i.e.* $c/a = 1$. These accidental lattice symmetries are special cases of *metrical pseudo-symmetries*. Owing to the anisotropy of the thermal expansion or the contraction under pressure, for special values of temperature and pressure singular lattice parameters may represent higher lattice symmetries than correspond to the symmetry of the crystal structure. The same may happen, and be much more pronounced, in continuous series of solid solutions owing to the change of cell dimensions with composition. Note that this phenomenon does not represent a new phase and a phase transition is not involved. Therefore, accidental lattice symmetries cannot be the basis for a classification in practice, *e.g.* for crystal structures or phase transitions. In contrast, *structural* pseudo-symmetries of crystals often lead to (displacive) phase transitions resulting in a new phase with higher structural *and* lattice symmetry.

In spite of its name, the classification of space groups into 'lattice systems of space groups' does *not* depend on the accidental symmetry of the translation lattice of a space group.

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