

## 8.2. CLASSIFICATIONS OF SPACE GROUPS, POINT GROUPS AND LATTICES

Thus, five Bravais types of lattices exist in  $E^2$ , and 14 in  $E^3$ . This classification can be transferred from vector lattices  $\mathbf{L}$  to point lattices  $L$ . To each point lattice  $L$  a vector lattice  $\mathbf{L}$  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  $\mathbf{L}$  of the space group  $\mathcal{G}$  may systematically have higher symmetry than the point group  $\mathcal{P}$  of  $\mathcal{G}$ . The lattice  $\mathbf{L}$ , 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  $\beta$  may be equal to  $91^\circ$ , whereas, for the same monoclinic crystal structure at some other temperature  $T_2$ ,  $\beta = 90^\circ$  may hold. In this case, the lattice  $\mathbf{L}$  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  $\mathbf{L}$  onto itself. The lattice  $\mathbf{L}$  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  $4I$ . 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  $a = b = c = 5 \text{ \AA}$ , 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  $R3$  and  $P6_1$  belong to the same crystal family because both  $R3$  and  $P3$  belong to the geometric crystal class 3, whereas both  $P3$  and  $P6_1$  are members of the same Bravais flock  $6/mmmP$ . In this example,  $P3$  serves as a link between  $R3$  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.