International Tables for Crystallography (2006). Vol. A, Section 8.2.3, pp. 727–728.

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

The symmetry of a vector lattice $\mathbf{L}$ is its point group according to the following definition:

Definition: The group $\mathcal{D}$ of *all* linear mappings which map a vector lattice $\mathbf{L}$ onto itself is called the *point group* or the *point symmetry of the lattice* $\mathbf{L}$. 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 $\mathbf{L}$, 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 $6mm$ but the point symmetry $\mathcal{D}$ of $\mathbf{L}$ is $6/mmm$. Thus, the point group $\mathcal{D}$ of the lattice $\mathbf{L}$ is of higher order than the point group $\mathcal{P}$ of $\mathcal{G}$.

Other symmetry operations of $\mathbf{L}$ 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 $\mathbf{L}$ than in the point group $\mathcal{P}$ of $\mathcal{G}$.

For purposes of classification, lattices $\mathbf{L}$ will now be considered independently of their space groups $\mathcal{G}$. Associated with each vector lattice $\mathbf{L}$ is a finite group $\mathcal{L}$ of $(n \times n)$ integral matrices which describes the point group $\mathcal{D}$ of $\mathbf{L}$ with respect to some primitive basis of $\mathbf{L}$. 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 $6mmP$. 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.

references