International Tables for Crystallography (2006). Vol. A1, Section 1.2.5.4, pp. 15–16.

The space groups are of different complexity. The simplest ones are the symmorphic space groups (not to be confused with 'isomorphic' space groups) according to the following definition:

Definition 1.2.5.3.5. A space group $\mathcal{G}$ is called *symmorphic* if representatives g_k of all cosets $\mathcal{T}(\mathcal{G})\,g_k$ can be found such that the set $\{g_k\}$ of all representatives forms a group. □

The group $\{g_k\}$ is finite and thus leaves a point F fixed. In the standard setting of any symmorphic space group such a point F is chosen as the origin. Thus, the translation parts of the elements g_k consist of zeroes only.

If a space group is symmorphic then all space groups of its type are symmorphic. Therefore, one can speak of 'symmorphic space-group types'. Symmorphic space groups can be recognized easily by their HM symbols: they contain an unmodified point-group symbol: rotations, reflections, inversions and rotoinversions but no screw rotations or glide reflections. There are 73 symmorphic space-group types of dimension three and 13 of dimension two; none of them show enantiomorphism.

One frequently speaks of 'the 230 space groups' or 'the 17 plane groups' and does not distinguish between the terms 'space group' and 'space-group type'. This is very often possible and is also done in this volume in order to make the explanations less long-winded. However, occasionally the distinction is indispensable in order to avoid serious difficulties of comprehension. For example, the sentence 'A space group is a proper subgroup of itself' is incomprehensible, whereas the sentence 'A space group and its proper subgroup belong to the same space-group type' makes sense.

1.2.5.4. *Point groups and crystal classes*

If the point coordinates are mapped by an isometry and its matrix–column pair, the vector coefficients are mapped by the linear part, *i.e.* by the matrix alone, *cf.* Section 1.2.2.6. Because the number of its elements is infinite, a space group generates from one point an infinite set of symmetry-equivalent points by its matrix–column pairs. Because the number of matrices of the linear parts is finite, the group of matrices generates from one vector a finite set of symmetry-equivalent vectors, *e.g.* the vectors normal to certain planes of the crystal. These planes determine the morphology of the ideal macroscopic crystal and its cleavage; the centre of the crystal represents the zero vector. When the symmetry of a crystal can only be determined by its macroscopic properties, only the symmetry group of the macroscopic crystal can be found. All its symmetry operations leave at least one point of the crystal fixed, *viz* its centre of mass. Therefore, this symmetry group was called the *point group of the crystal*, although its symmetry operations are those of vector space, not of point space. Although misunderstandings are not rare, this name is still used in today's crystallography for historical reasons.[7]

Let a conventional coordinate system be chosen and the elements $g_j \in \mathcal{G}$ be represented by the matrix–column pairs $(\boldsymbol{W}_j, \boldsymbol{w}_j)$, with the representation of the translations $t_k \in \mathcal{T}(\mathcal{G})$ by the pairs $(\boldsymbol{I}, \boldsymbol{t}_k)$. Then the composition of $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ with all translations forms an infinite set $\{(\boldsymbol{I}, \boldsymbol{t}_k)(\boldsymbol{W}_j, \boldsymbol{w}_j) = (\boldsymbol{W}_j, \boldsymbol{w}_j + \boldsymbol{t}_k)\}$ of symmetry operations which is a right coset of the coset decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$. From this equation it follows that the elements of the same coset of the decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ have the same linear part. On the other hand, elements of different cosets have different linear parts if $\mathcal{T}(\mathcal{G})$ contains all translations of $\mathcal{G}$. Thus, each coset can be characterized by its linear part. It can be shown from equations (1.2.2.5) and (1.2.2.6) that the linear parts form a group which is isomorphic to the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, *i.e.* to the group of the cosets.

Definition 1.2.5.4.1. A group of linear parts, represented by a group of matrices $\boldsymbol{W}_j$, is called a *point group* $\mathcal{P}$. If the linear parts are those of the matrix–column pairs describing the symmetry operations of a space group $\mathcal{G}$, the group is called the *point group* $\mathcal{P}_{\mathcal{G}}$ of the space group $\mathcal{G}$. The point groups that can belong to space groups are called *crystallographic point groups*. □

According to Definition 1.2.5.4.1, the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is isomorphic to the point group $\mathcal{P}_{\mathcal{G}}$. This property is exploited in the graphs of *translationengleiche* subgroups of space groups, *cf.* Chapter 2.4 and Section 2.1.7.2.

All point groups in the following sections are crystallographic point groups. The maximum order of a crystallographic point group is 48 in three-dimensional space and 12 in two-dimensional space.

As with space groups, there are also an infinite number of crystallographic point groups which may be classified into a finite number of point-group types. This cannot be done by isomorphism because geometrically different point groups may be isomorphic. For example, point groups consisting of the identity with the inversion $\{\boldsymbol{I}, \overline{\boldsymbol{I}}\}$ or with a twofold rotation $\{\boldsymbol{I}, \boldsymbol{2}\}$ or with a reflection through a plane $\{\boldsymbol{I}, \boldsymbol{m}\}$ are all isomorphic to the (abstract) group of order 2. As for space groups, the classification may be performed, however, referring the point groups to corresponding vector bases. As translations do not occur among the point-group operations, one may choose any basis for the description of the symmetry operations by matrices. One takes the basis of $\{\boldsymbol{W}'\}$ as given and transforms the basis of $\{\boldsymbol{W}\}$ to the basis corresponding to that of $\{\boldsymbol{W}'\}$. This leads to the definition:

Definition 1.2.5.4.2. Two crystallographic point groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}'_{\mathcal{G}'}$ belong to the same *point-group type* or to the same *crystal class of point groups* if there is a real non-singular matrix $\boldsymbol{P}$ which maps a matrix group $\{\boldsymbol{W}\}$ of $\mathcal{P}_{\mathcal{G}}$ onto a matrix group $\{\boldsymbol{W}'\}$ of $\mathcal{P}'_{\mathcal{G}'}$ by the transformation $\{\boldsymbol{W}'\} = \boldsymbol{P}^{-1}\,\{\boldsymbol{W}\}\,\boldsymbol{P}$. □

Point groups can be classified by Definition 1.2.5.4.2. Further space groups may be classified into 'crystal classes of space groups' according to their point groups:

Definition 1.2.5.4.3. Two space groups belong to the same *crystal class of space groups* if their point groups belong to the same crystal class of point groups. □

Whether two space groups belong to the same crystal class or not can be worked out from their standard HM symbols: one removes the lattice parts from these symbols as well as the constituents '1' from the symbols of trigonal space groups and replaces all constituents for screw rotations and glide reflections by those for the corresponding pure rotations and reflections. The symbols obtained in this way are those of the corresponding point groups. If they agree, the space groups belong to the same crystal class. The space groups also belong to the same crystal class if the point-group symbols belong to the pair $\overline{4}2m$ and $\overline{4}m2$ or to the pair $\overline{6}2m$ and $\overline{6}m2$.

There are 32 classes of three-dimensional crystallographic point groups and 32 crystal classes of space groups, and ten classes of two-dimensional crystallographic point groups and ten crystal classes of plane groups.

The distribution into crystal classes classifies space-group types – and thus space groups – and crystallographic point groups. It

[7] The term *point group* is also used for a group of symmetry operations of point space, which is better called a *site-symmetry group* and which is the group describing the symmetry of the surroundings of a point in point space.

does not classify the infinite set of all lattices into a finite number of lattice types, because the same lattice may belong to space groups of different crystal classes. For example, the same lattice may be that of a space group of type $P1$ (of crystal class 1) and that of a space group of type $P\overline{1}$ (of crystal class $\overline{1}$).

Nevertheless, there is also a definition of the 'point group of a lattice'. Let a vector lattice **L** of a space group $\mathcal{G}$ be referred to a lattice basis. Then the linear parts $\boldsymbol{W}$ of the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ of $\mathcal{G}$ form the point group $\mathcal{P}_{\mathcal{G}}$. If $(\boldsymbol{W}, \boldsymbol{w})$ maps the space group $\mathcal{G}$ onto itself, then the linear part $\boldsymbol{W}$ maps the (vector) lattice **L** onto itself. However, there may be additional matrices which also describe symmetry operations of the lattice **L**. For example, the point group $\mathcal{P}_{\mathcal{G}}$ of a space group of type $P1$ consists of the identity $\boldsymbol{I}$ only. However, with any vector $\mathbf{t} \in \mathbf{L}$, the negative vector $-\mathbf{t} \in \mathbf{L}$ also belongs to **L**. Therefore, the lattice **L** is always centrosymmetric and has the inversion $\overline{\boldsymbol{I}}$ as a symmetry operation independent of the symmetry of the space group.

Definition 1.2.5.4.4. The set of all orthogonal mappings with matrices $\boldsymbol{W}$ which map a lattice **L** onto itself is called the point group of the lattice **L** or the *holohedry* of the lattice **L**. A crystal class of point groups $\mathcal{P}_{\mathcal{G}}$ is called a *holohedral crystal class* if it contains a holohedry. □

There are seven holohedral crystal classes in the space: $\overline{1}$, $2/m$, mmm, $4/mmm$, $\overline{3}m$, $6/mmm$ and $m\overline{3}m$. Their lattices are called triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal and cubic, respectively. There are four holohedral crystal classes in the plane: 2, $2mm$, $4mm$ and $6mm$. Their two-dimensional lattices (or nets) are called oblique, rectangular, square and hexagonal, respectively.

The lattices can be classified into *lattice types* or *Bravais types*, mostly called *Bravais lattices*, or into *lattice systems* (called *Bravais systems* in editions 1 to 4 of *IT* A). These classifications are not discussed here because they are not directly relevant to the classification of the space groups. This is because the lattice symmetry is not necessarily typical for the symmetry of its space group but may accidentally be higher. For example, the lattice of a monoclinic crystal may be accidentally orthorhombic (only for certain values of temperature and pressure). In Sections 8.2.5 and 8.2.7 of *IT* A the 'typical lattice symmetry' of a space group is defined.

1.2.5.5. *Crystal systems and crystal families*

The example of $P1$ mentioned above shows that the point group of the lattice may be systematically of higher order than that of its space group. There are obviously point groups and thus space groups that belong to a holohedral crystal class and those that do not. The latter can be assigned to a holohedral crystal class uniquely according to the following definition:[8]

Definition 1.2.5.5.1. A crystal class **C** of a space group $\mathcal{G}$ is either holohedral **H** or it can be assigned uniquely to **H** by the condition: any point group of **C** is a subgroup of a point group of **H** but not a subgroup of a holohedral crystal class **H′** of smaller order. The set of all crystal classes of space groups that are assigned to the same holohedral crystal class is called a *crystal system* of space groups. □

The 32 crystal classes of space groups are classified into seven crystal systems which are called *triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic*. There are four crystal systems of plane groups: *oblique, rectangular, square and hexagonal*. Like the space groups, the crystal classes of point groups are classified into the seven crystal systems of point groups.

Apart from accidental lattice symmetries, the space groups of different crystal systems have lattices of different symmetry. As an exception, the hexagonal primitive lattice occurs in both hexagonal and trigonal space groups as the typical lattice. Therefore, the space groups of the trigonal and the hexagonal crystal systems are more related than space groups from other different crystal systems. Indeed, in different crystallographic schools the term 'crystal system' was used for different objects. One sense of the term was the 'crystal system' as defined above, while another sense of the old term 'crystal system' is now called a 'crystal family' according to the following definition [for definitions that are also valid in higher-dimensional spaces, see Brown *et al.* (1978) or *IT* A, Chapter 8.2]:

Definition 1.2.5.5.2. In three-dimensional space, the classification of the set of all space groups into crystal families is the same as that into crystal systems with the one exception that the trigonal and hexagonal crystal systems are united to form the *hexagonal crystal family*. There is no difference between crystal systems and crystal families in the plane. □

The partition of the space groups into crystal families is the most universal one. The space groups and their types, their crystal classes and their crystal systems are classified by the crystal families. Analogously, the crystallographic point groups and their crystal classes and crystal systems are classified by the crystal families of point groups. Lattices, their Bravais types and lattice systems can also be classified into crystal families of lattices; *cf. IT* A, Chapter 8.2.

1.2.6. Types of subgroups of space groups

1.2.6.1. *Introductory remarks*

Group–subgroup relations form an essential part of the applications of space-group theory. Let $\mathcal{G}$ be a space group and $\mathcal{H} < \mathcal{G}$ a proper subgroup of $\mathcal{G}$. All maximal subgroups $\mathcal{H} < \mathcal{G}$ of any space group $\mathcal{G}$ are listed in Part 2 of this volume. There are different kinds of subgroups which are defined and described in this section. The tables and graphs of this volume are arranged according to these kinds of subgroups. Moreover, for the different kinds of subgroups different data are listed in the subgroup tables and graphs.

Let $\mathcal{G}_j$ and $\mathcal{H}_j$ be space groups of the space-group types $\mathcal{G}$ and $\mathcal{H}$. The group–subgroup relation $\mathcal{G}_j > \mathcal{H}_j$ is a relation between the particular space groups $\mathcal{G}_j$ and $\mathcal{H}_j$ but it can be generalized to the space-group types $\mathcal{G}$ and $\mathcal{H}$. Certainly, not every space group of the type $\mathcal{H}$ will be a subgroup of every space group of the type $\mathcal{G}$. Nevertheless, the relation $\mathcal{G}_j > \mathcal{H}_j$ holds for any space group of $\mathcal{G}$ and $\mathcal{H}$ in the following sense: If $\mathcal{G}_j > \mathcal{H}_j$ holds for the pair $\mathcal{G}_j$ and $\mathcal{H}_j$, then for any space group $\mathcal{G}_k$ of the type $\mathcal{G}$ a space group $\mathcal{H}_k$ of the type $\mathcal{H}$ exists for which the corresponding relation $\mathcal{G}_k > \mathcal{H}_k$ holds. Conversely, for any space group $\mathcal{H}_m$ of the type $\mathcal{H}$ a space group $\mathcal{G}_m$ of the type $\mathcal{G}$ exists for which the corresponding relation $\mathcal{G}_m > \mathcal{H}_m$ holds. Only this property of the group–subgroup relations made it possible to compile and arrange the tables of this volume so that they are as concise as those of *IT* A.

1.2.6.2. *Definitions and examples*

'Maximal subgroups' have been introduced by Definition 1.2.4.1.2. The importance of this definition will become apparent

[8] This assignment does hold for low dimensions of space at least up to dimension 4. A dimension-independent definition of the concepts of 'crystal system' and 'crystal family' is found in *IT* A, Chapter 8.2, where the classifications are treated in more detail.

references