International Tables for Crystallography (2011). Vol. A1, Section 1.2.5.5, pp. 17–18.

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 $\{\boldsymbol{I}, \bar{\boldsymbol{I}}\}$ 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 $\bar{4}2m$ and $\bar{4}m2$ or to the pair $\bar{6}2m$ and $\bar{6}m2$.

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 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 $P\bar{1}$ (of crystal class $\bar{1}$).

Nevertheless, there is also a definition of the 'point group of a lattice'. Let a vector lattice $\mathbf{L}$ 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 $\mathbf{L}$ onto itself. However, there may be additional matrices which also describe symmetry operations of the lattice $\mathbf{L}$. 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 $\mathbf{L}$. Therefore, the lattice $\mathbf{L}$ is always centrosymmetric and has the inversion $\bar{\boldsymbol{I}}$ 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 $\mathbf{L}$ onto itself is called the point group of the lattice $\mathbf{L}$ or the *holohedry* of the lattice $\mathbf{L}$. 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: $\bar{1}$, $2/m$, mmm, $4/mmm$, $\bar{3}m$, $6/mmm$ and $m\bar{3}m$. 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:[9]

Definition 1.2.5.5.1. A crystal class $\mathbf{C}$ of a space group $\mathcal{G}$ is either holohedral $\mathbf{H}$ or it can be assigned uniquely to $\mathbf{H}$ by the condition: any point group of $\mathbf{C}$ is a subgroup of a point group of $\mathbf{H}$ but not a subgroup of a holohedral crystal class $\mathbf{H}'$ 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

[9] This assignment does hold for low dimensions of space 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.

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 in the corollary to Hermann's theorem, *cf.* Lemma 1.2.8.1.3. In this volume only the maximal subgroups are listed for any plane and any space group. A maximal subgroup of a plane group is a plane group, a maximal subgroup of a space group is a space group. On the other hand, a minimal supergroup of a plane group or of a space group is not necessarily a plane group or a space group, *cf.* Section 2.1.6.

If the maximal subgroups are known for each space group, then each non-maximal subgroup of a space group $\mathcal{G}$ with finite index can in principle be obtained from the data on maximal subgroups. A non-maximal subgroup $\mathcal{H} < \mathcal{G}$ of finite index $[i]$ is connected with the original group $\mathcal{G}$ through a chain $\mathcal{H} = \mathcal{Z}_k < \mathcal{Z}_{k-1} < \ldots < \mathcal{Z}_1 < \mathcal{Z}_0 = \mathcal{G}$, where each group $\mathcal{Z}_j < \mathcal{Z}_{j-1}$ is a maximal subgroup of $\mathcal{Z}_{j-1}$, with the index $[i_j] = |\mathcal{Z}_{j-1} : \mathcal{Z}_j|$, $j = 1, \ldots, k$. The number k is finite and the relation $i = \prod_{j=1}^{k} i_j$ holds, *i.e.* the total index $[i]$ is the product of the indices i_j.

According to Hermann (1929), the following types of subgroups of space groups have to be distinguished:

Definition 1.2.6.2.1. A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is called a *translationengleiche subgroup* or a *t*-subgroup of $\mathcal{G}$ if the set $\mathcal{T}(\mathcal{G})$ of translations is retained, *i.e.* $\mathcal{T}(\mathcal{H}) = \mathcal{T}(\mathcal{G})$, but the number of cosets of $\mathcal{G}/\mathcal{T}(\mathcal{G})$, *i.e.* the order P of the point group $\mathcal{P}_{\mathcal{G}}$, is reduced such that $|\mathcal{G}/\mathcal{T}(\mathcal{G})| > |\mathcal{H}/\mathcal{T}(\mathcal{H})|$.[10] □

The order of a crystallographic point group $\mathcal{P}_{\mathcal{G}}$ of the space group $\mathcal{G}$ is always finite. Therefore, the number of the subgroups of $\mathcal{P}_{\mathcal{G}}$ is also always finite and these subgroups and their relations are displayed in well known graphs, *cf.* Chapter 2.4 and Section 2.1.8 of this volume. Because of the isomorphism between the point group $\mathcal{P}_{\mathcal{G}}$ and the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, the subgroup graph for the point group $\mathcal{P}_{\mathcal{G}}$ is the same as that for the *t*-subgroups of $\mathcal{G}$, only the labels of the groups are different. For deviations between the point-group graphs and the actual space-group graphs of Chapter 2.4, *cf.* Section 2.1.8.2.

Example 1.2.6.2.2

Consider a space group $\mathcal{G}$ of type $P12/m1$ referred to a conventional coordinate system. The translation subgroup $\mathcal{T}(\mathcal{G})$ consists of all translations with translation vectors $\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, where u, v, w run through all integer numbers. The coset decomposition of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ results in the four cosets $\mathcal{T}(\mathcal{G})$, $\mathcal{T}(\mathcal{G})\,\boldsymbol{2}_0$, $\mathcal{T}(\mathcal{G})\,\boldsymbol{m}_0$ and $\mathcal{T}(\mathcal{G})\,\bar{\boldsymbol{1}}_0$, where the right operations are a twofold rotation $\boldsymbol{2}_0$ around the rotation axis passing through the origin, a reflection $\boldsymbol{m}_0$ through a plane containing the origin and an inversion $\bar{\boldsymbol{1}}_0$ with the inversion point at the origin, respectively. The three combinations $\mathcal{H}_1 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\,\boldsymbol{2}_0$, $\mathcal{H}_2 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\,\boldsymbol{m}_0$ and $\mathcal{H}_3 = \mathcal{T}(\mathcal{G}) \cup (\mathcal{T}\mathcal{G})\,\bar{\boldsymbol{1}}_0$ each form a *translationengleiche* maximal subgroup of $\mathcal{G}$ of index 2 with the space-group symbols $P121$, $P1m1$ and $P\bar{1}$, respectively.

Definition 1.2.6.2.3. A subgroup $\mathcal{H} < \mathcal{G}$ of a space group $\mathcal{G}$ is called a *klassengleiche subgroup* or a *k-subgroup* if the set $\mathcal{T}(\mathcal{G})$ of all translations of $\mathcal{G}$ is reduced to $\mathcal{T}(\mathcal{H}) < \mathcal{T}(\mathcal{G})$ but all linear parts of $\mathcal{G}$ are retained. Then the number of cosets of the decompositions $\mathcal{H}/\mathcal{T}(\mathcal{H})$ and $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is the same, *i.e.* $|\mathcal{H}/\mathcal{T}(\mathcal{H})| = |\mathcal{G}/\mathcal{T}(\mathcal{G})|$. In other words: the order of the point group $\mathcal{P}_{\mathcal{H}}$ is the same as that of $\mathcal{P}_{\mathcal{G}}$. See also footnote 10. □

For a *klassengleiche* subgroup $\mathcal{H} < \mathcal{G}$, the cosets of the factor group $\mathcal{H}/\mathcal{T}(\mathcal{H})$ are smaller than those of $\mathcal{G}/\mathcal{T}(\mathcal{G})$. Because $\mathcal{T}(\mathcal{H})$ is still infinite, the number of elements of each coset is infinite but the index $|\mathcal{T}(\mathcal{G}) : \mathcal{T}(\mathcal{H})| > 1$ is finite. The number of *k*-subgroups of $\mathcal{G}$ is always infinite.

[10] German: *zellengleiche* means 'with the same cell'; *translationengleiche* means 'with the same translations'; *klassengleiche* means 'of the same (crystal) class'. Of the different German declension endings only the form with terminal *-e* is used in this volume. The terms *zellengleiche* and *klassengleiche* were introduced by Hermann (1929). The term *zellengleiche* was later replaced by *translationengleiche* because of possible misinterpretations. In this volume they are sometimes abbreviated as *t*-subgroups and *k*-subgroups.

references