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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.

Example 1.2.6.2.4

Consider a space group $\mathcal{G}$ of the type $C121$, referred to a conventional coordinate system. The set $\mathcal{T}(\mathcal{G})$ of all translations can be split into the set $\mathcal{T}_i$ of all translations with integer coefficients u, v and w and the set $\mathcal{T}_f$ of all translations for which the coefficients u and v are fractional. The set $\mathcal{T}_i$ forms a group; the set $\mathcal{T}_f$ is the other coset in the decomposition $(\mathcal{T}(\mathcal{G}) : \mathcal{T}_i)$ and does not form a group. Let t_C be the 'centring translation' with the translation vector $\frac{1}{2}(\mathbf{a}+\mathbf{b})$. Then $\mathcal{T}_f$ can be written $\mathcal{T}_i\, t_C$. Let $\boldsymbol{2}_0$ mean a twofold rotation around the rotation axis through the origin. There are altogether four cosets of the decomposition $(\mathcal{G} : \mathcal{T}_i)$, which can be written now as $\mathcal{T}_i$, $\mathcal{T}_f = \mathcal{T}_i\, t_C$, $\mathcal{T}_i\, \boldsymbol{2}_0$ and $\mathcal{T}_f\, \boldsymbol{2}_0 = (\mathcal{T}_i\, t_C)\, \boldsymbol{2}_0 = \mathcal{T}_i\, (t_C\, \boldsymbol{2}_0)$. The union $\mathcal{T}_i \cup (\mathcal{T}_i\, t_C) = \mathcal{T}_{\mathcal{G}}$ forms the *translationengleiche* maximal subgroup $C1$ (conventional setting $P1$) of $\mathcal{G}$ of index 2. The union $\mathcal{T}_i \cup (\mathcal{T}_i\, \boldsymbol{2}_0)$ forms the *klassengleiche* maximal subgroup $P121$ of $\mathcal{G}$ of index 2. The union $\mathcal{T}_i \cup (\mathcal{T}_i (t_C\, \boldsymbol{2}_0))$ also forms a *klassengleiche* maximal subgroup of index 2. Its HM symbol is $P12_11$, and the twofold rotations $\boldsymbol{2}$ of the point group $\boldsymbol{2}$ are realized by screw rotations $\boldsymbol{2}_1$ in this subgroup because $(t_C\, \boldsymbol{2}_0)$ is a screw rotation with its screw axis running parallel to the $\mathbf{b}$ axis through the point $\frac{1}{4}, 0, 0$. There are in fact these two k-subgroups of $C121$ of index 2 which have the group $\mathcal{T}_i$ in common. In the subgroup table of $C121$ both are listed under the heading 'Loss of centring translations' because the conventional unit cell is retained while only the centring translations have disappeared. (Four additional *klassengleiche* maximal subgroups of $C121$ with index 2 are found under the heading 'Enlarged unit cell'.)

The group $\mathcal{T}_i$ of type $P1$ is a non-maximal subgroup of $C121$ of index 4.

Definition 1.2.6.2.5. A *klassengleiche* or k-subgroup $\mathcal{H} < \mathcal{G}$ is called *isomorphic* or an *isomorphic subgroup* if it belongs to the same affine space-group type (isomorphism type) as $\mathcal{G}$. If a subgroup is not isomorphic, it is sometimes called *non-isomorphic*. □

Isomorphic subgroups are special k-subgroups. The importance of the distinction between k-subgroups in general and isomorphic subgroups in particular stems from the fact that the number of maximal non-isomorphic k-subgroups of any space group is finite, whereas the number of maximal isomorphic subgroups is always infinite, see Section 1.2.8.

Example 1.2.6.2.6

Consider a space group $\mathcal{G}$ of type $P\overline{1}$ 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 and w run through all integer numbers. There is an inversion $\overline{\boldsymbol{1}}_0$ with the inversion point at the origin and also an infinite number of other inversions, generated by the combinations of $\overline{\boldsymbol{1}}_0$ with all translations of $\mathcal{T}(\mathcal{G})$.

We consider the subgroup $\mathcal{T}_g$ of all translations with an even coefficient u and arbitrary integers v and w as well as the coset decomposition $(\mathcal{G} : \mathcal{T}_g)$. Let t_a be the translation with the translation vector $\mathbf{a}$. There are four cosets: $\mathcal{T}_g$, $\mathcal{T}_g\, t_a$, $\mathcal{T}_g\, \overline{\boldsymbol{1}}_0$ and $\mathcal{T}_g (t_a\, \overline{\boldsymbol{1}}_0)$. The union $\mathcal{T}_g \cup (\mathcal{T}_g\, t_a)$ forms the *translationengleiche* maximal subgroup $\mathcal{T}(\mathcal{G})$ of index 2. The union $\mathcal{T}_g \cup (\mathcal{T}_g\, \overline{\boldsymbol{1}}_0)$ forms an isomorphic maximal subgroup of index 2, as does the union $\mathcal{T}_g \cup (\mathcal{T}_g\, (t_a\, \overline{\boldsymbol{1}}_0))$. There are thus two maximal isomorphic subgroups of index 2 which are obtained by doubling the a lattice parameter. There are altogether 14 isomorphic subgroups of index 2 for any space group of type $P\overline{1}$ which are obtained by seven different cell enlargements.

If $\mathcal{G}$ belongs to a pair of enantiomorphic space-group types, then the isomorphic subgroups of $\mathcal{G}$ may belong to different crystallographic space-group types with different HM symbols and different space-group numbers. In this case, an infinite number of subgroups belong to the crystallographic space-group type of $\mathcal{G}$ and another infinite number belong to the enantiomorphic space-group type.

Example 1.2.6.2.7

Space group $P4_1$, No. 76, has for any prime number $p > 2$ an isomorphic maximal subgroup of index p with the lattice parameters a, b, pc. This is an infinite number of subgroups because there is an infinite number of primes. The subgroups belong to the space-group type $P4_1$ if $p = 4n + 1$; they belong to the type $P4_3$ if $p = 4n + 3$.

Definition 1.2.6.2.8. A subgroup of a space group is called *general* or a *general subgroup* if it is neither a *translationengleiche* nor a *klassengleiche* subgroup. It has lost translations as well as linear parts, *i.e.* point-group symmetry. □

Example 1.2.6.2.9

The subgroup $\mathcal{T}_g$ in Example 1.2.6.2.6 has lost all inversions of the original space group $P\overline{1}$ as well as all translations with odd u. It is a general subgroup $P1$ of the space group $P\overline{1}$ of index 4.

1.2.6.3. The role of normalizers for group–subgroup pairs of space groups

In Section 1.2.4.5, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of a subgroup $\mathcal{H} < \mathcal{G}$ in the group $\mathcal{G}$ was defined. The equation $\mathcal{H} \trianglelefteq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \le \mathcal{G}$ holds, *i.e.* $\mathcal{H}$ is a normal subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$, by its index in $\mathcal{G}$, determines the number $N_j = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$ of subgroups $\mathcal{H}_j < \mathcal{G}$ that are conjugate in the group $\mathcal{G}$, *cf.* Remarks (2) and (3) below Definition 1.2.4.5.1.

The group–subgroup relations between space groups become more transparent if one looks at them from a more general point of view. Space groups are part of the general theory of mappings. Particular groups are the *affine group* $\mathcal{A}$ of all reversible affine mappings, the *Euclidean group* $\mathcal{E}$ of all isometries, the *translation group* $\mathcal{T}$ of all translations and the *orthogonal group* $\mathcal{O}$ of all orthogonal mappings.

Connected with any particular space group $\mathcal{G}$ are its group of translations $\mathcal{T}(\mathcal{G})$ and its point group $\mathcal{P}_{\mathcal{G}}$. In addition, the normalizers $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of $\mathcal{G}$ in the affine group $\mathcal{A}$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ in the Euclidean group $\mathcal{E}$ are useful. They are listed in Section 15.2.1 of *IT* A. Although consisting of isometries only, $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is not necessarily a space group, see the second paragraph of Example 1.2.7.3.1.

For the group–subgroup pairs $\mathcal{H} < \mathcal{G}$ the following relations hold:

(1) $\mathcal{T}(\mathcal{H}) \le \mathcal{H} \le \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \le \mathcal{G} \le \mathcal{N}_{\mathcal{E}}(\mathcal{G}) < \mathcal{E}$;

(1a) $\mathcal{H} \le \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \le \mathcal{N}_{\mathcal{E}}(\mathcal{H}) < \mathcal{E}$;

(1b) $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) \le \mathcal{N}_{\mathcal{A}}(\mathcal{H}) < \mathcal{A}$;

(2) $\mathcal{T}(\mathcal{H}) \le \mathcal{T}(\mathcal{G}) < \mathcal{T} < \mathcal{E}$;

(3) $\mathcal{T}(\mathcal{G}) \le \mathcal{G} \le \mathcal{N}_{\mathcal{E}}(\mathcal{G}) \le \mathcal{N}_{\mathcal{A}}(\mathcal{G}) < \mathcal{A}$.

The subgroup $\mathcal{H}$ may be a *translationengleiche* or a *klassengleiche* or a general subgroup of $\mathcal{G}$. In any case, the normalizer

references