1.7. Topics on space groups treated in Volumes A1 and E of *International Tables for Crystallography*

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1.7.1. Subgroups and supergroups of space groups

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Relations between crystal structures play an important role for the comparison and classification of crystal structures, the analysis of phase transitions in the solid state, the understanding of topotactic reactions, and other applications. The relations can often be expressed by group–subgroup relations between the corresponding space groups. Such relations may be recognized from relations between the lattices and between the point groups[1] of the crystal structures.

In the first five editions of this Volume A of *International Tables for Crystallography*, subgroups and those supergroups of space groups that are space groups were listed for every space group. However, the listing was incomplete and it lacked additional information, such as, for example, possible unit-cell transformations and/or origin shifts involved. It became apparent that complete lists and more detailed data were necessary. Therefore, a supplementary volume of *International Tables for Crystallography* to this Volume A has been published: Volume A1, *Symmetry Relations between Space Groups* (2004; second edition 2010), abbreviated as *IT* A1 in this chapter. The listing of the subgroups and supergroups has thus been discontinued in this sixth edition of Volume A.

This chapter gives a short outline of the contents and applications of the relations listed in Volume A1. In addition, information on Volume E of *International Tables for Crystallography* is presented. Volume E lists the subperiodic groups, which are other kinds of subgroups of the space groups.

Volume A1 consists of three parts. Part 1 covers the theory of space groups and their subgroups, space-group relations between crystal structures and the corresponding Wyckoff positions, and the Bilbao Crystallographic Server (http://www.cryst.ehu.es/). This server is freely accessible and offers access to computer programs that display the subgroups and supergroups of the space groups and other relevant data. Part 2 of Volume A1 contains complete lists of the maximal subgroups of the plane groups and space groups, including unit-cell transformations and origin shifts, if applicable. An overview of the group–subgroup relations is also displayed in diagrams. Part 3 contains tables of relations between the Wyckoff positions of group–subgroup-related space groups and a guide to their use.

Example

The crystal structures of silicon, Si, and sphalerite, ZnS, belong to space-group types $Fd\bar{3}m$ (O_h^7; No. 227) and $F\bar{4}3m$ (T_d^2; No. 216) with lattice parameters $a_{\rm Si}$ = 5.43 Å and $a_{\rm ZnS}$ = 5.41 Å. The structure of sphalerite (zinc blende) is obtained from that of silicon by replacing alternately half of the Si atoms by Zn and half by S, and by adjusting the lattice parameter. This procedure is described in detail in Fig. 1.7.2.1. The strong connection between the two crystal structures is reflected in the relation between their space groups: the point group (crystal class) and the space group of sphalerite is a subgroup (of index 2) of that of silicon (ignoring the small difference in lattice parameters).

Data on subgroups and supergroups of the space groups are useful for the discussion of structural relations and phase transitions. It must be kept in mind, however, that group–subgroup relations only constitute symmetry relations. It is important, therefore, to ascertain that the consequential relations between the lattice parameters and between the atomic coordinates of the particles of the crystal structures also hold before a structural relation can be deduced from a symmetry relation.

Examples

NaCl and CaF_2 belong to the same space-group type, $Fm\bar{3}m$ (O_h^5; No. 225), and have lattice parameters $a_{\rm NaCl}$ = 5.64 Å and $a_{\rm CaF_2}$ = 5.46 Å. The ions, however, occupy unrelated positions and so the symmetry relation does not express a structural relation.

Pyrite, FeS_2, and solid carbon dioxide, CO_2, belong to the same space-group type, $Pa\bar{3}$ (T_h^6; No. 205). They have lattice parameters $a_{\rm FeS_2}$ = 5.42 Å and $a_{\rm CO_2}$ = 5.55 Å, and the particles occupy analogous Wyckoff positions. Nevertheless, the structures of these compounds are not related, because the positional parameters $x = 0.386$ of S in FeS_2 and $x = 0.118$ of O in CO_2 differ so much that the coordinations of the corresponding atoms are dissimilar.

To formulate group–subgroup relations some definitions are necessary. Subgroups and their distribution into conjugacy classes, normal subgroups, supergroups, maximal subgroups, minimal supergroups, proper subgroups, proper supergroups and index are defined for groups in general in Chapter 1.1. These definitions are used also for crystallographic groups like space groups. In the present chapter, the data of *IT* A1 are explained through many examples in order to enable the reader to use *IT* A1.

Examples

Maximal subgroups $\mathcal{H}$ of a space group $P1$ with basis vectors **a**, **b**, **c** are, among others, subgroups $P1$ for which $\mathbf{a}'' = p\mathbf{a}$, $\mathbf{b}'' = \mathbf{b}$, $\mathbf{c}'' = \mathbf{c}$, p prime. If p is not a prime number but a product of two integers $p = q \times r$, the subgroup $\mathcal{H}$ is not maximal because a proper subgroup $\mathcal{Z}$ of index q exists such that $\mathbf{a}' = qa$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$. $\mathcal{Z}$ again has $\mathcal{H}$ as a proper subgroup of index r with $\mathcal{G} > \mathcal{Z} > \mathcal{H}$.

$P12_1/c1$ has maximal subgroups $P12_11$, $P1c1$ and $P\bar{1}$ with the same unit cell, whereas $P1$ is not a maximal subgroup of $P12_1/c1$: $P12_1/c1 > P12_11 > P1$; $P12_1/c1 > P1c1 > P1$; $P12_1/c1 > P\bar{1} > P1$. These are all possible chains of maximal subgroups for $P12_1/c1$ if the original translations are retained

[1] The point group determines both the symmetry of the physical properties of the macroscopic crystal and the symmetry of its ideal shape. Each space group belongs to a point group.

completely. Correspondingly, the seven subgroups of index 4 with the same translations as the original space group $P6_3/mcm$ are obtained *via* the 21 different chains of Fig. 1.7.1.1.

While all group–subgroup relations considered here are relations between individual space groups, they are valid for all space groups of a space-group type, as the following example shows.

Example

A particular space group $P121$ has a subgroup $P1$ which is obtained from $P121$ by retaining all translations but eliminating all rotations and combinations of rotations with translations. For every space group of space-group type $P121$ such a subgroup $P1$ exists.

From this example it follows that the relationship exists, in an extended sense, for the two space-group types involved. One can, therefore, list these relationships by means of the symbols of the space-group types.

A three-dimensional space group may have subgroups with no translations (*i.e.* site-symmetry groups; *cf.* Section 1.4.5), or with one- or two-dimensional lattices of translations (*i.e.* line groups, frieze groups, rod groups, plane groups and layer groups), *cf.* Volume E of *International Tables for Crystallography*, or with a three-dimensional lattice of translations (space groups).

The number of subgroups of a space group is always infinite. Not only the number of all subgroups but even the number of all maximal subgroups of a given space group is infinite.

In this section, only those subgroups of a space group that are also space groups will be considered. All *maximal* subgroups of space groups are themselves space groups. To simplify the discussion, let us suppose that we know all maximal subgroups of a space group $\mathcal{G}$. In this case, *any* subgroup $\mathcal{H}$ of $\mathcal{G}$ may be obtained *via* a chain of maximal subgroups $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_{r-1}, \mathcal{H}_r$ such that $\mathcal{G}\ (= \mathcal{H}_0) > \mathcal{H}_1 > \mathcal{H}_2 > \ldots > \mathcal{H}_{r-1} > \mathcal{H}_r\ (= \mathcal{H})$, where $\mathcal{H}_j$ is a maximal subgroup of $\mathcal{H}_{j-1}$ of index $[i_j]$, with $j = 1, \ldots, r$. There may be many such chains between $\mathcal{G}$ and $\mathcal{H}$. On the other hand, all subgroups of $\mathcal{G}$ of a given index $[i]$ are obtained if all chains are constructed for which $[i_1] \times [i_2] \times \ldots \times [i_r] = [i]$ holds.

The index $[i]$ of a subgroup has a geometric significance. It determines the 'dilution' of symmetry operations of $\mathcal{H}$ compared with those of $\mathcal{G}$. The number of symmetry operations of $\mathcal{H}$ is $1/i$ times the number of symmetry operations of $\mathcal{G}$; since space groups are infinite groups, this is to be understood in the same way as 'the number of even numbers is one half of the number of all integer numbers'.

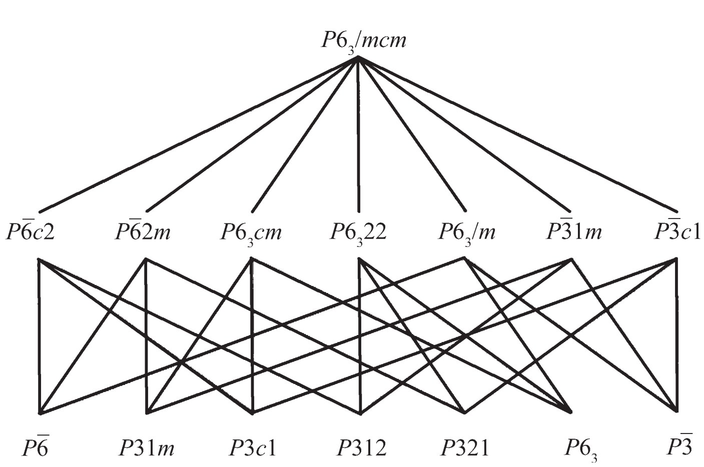

Figure 1.7.1.1
Space group $P6_3/mcm$ with t-subgroups of index 2 and 4. All 21 possible subgroup chains are displayed by lines.

The infinite number of subgroups only occurs for a certain kind of subgroup and can be reduced as described below. It is thus useful to consider the different kinds of subgroups of a space group in the way introduced by Hermann (1929):

(1) By reducing the order of the point group, *i.e.* by eliminating all symmetry operations of some kind. The example $P12_11 \longrightarrow P1$ mentioned above is of this type;
(2) By loss of translations, *i.e.* by 'thinning out' the lattice of translations. For the space group $P121$ mentioned above this may happen in different ways:
   (*a*) by suppressing all translations of the kind $(2u+1)\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, where u, v and w are integers. The new basis is normally written $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$ and, hence, half of the twofold axes have been eliminated; or
   (*b*) by $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, *i.e.* by thinning out the translations parallel to the twofold axes; or
   (*c*) again by $\mathbf{b}' = 2\mathbf{b}$ but replacing the twofold rotation axes by twofold screw axes.
(3) By combination of (1) and (2), *e.g.* by reducing the order of the point group and by thinning out the lattice of translations.

Subgroups of the first kind, (1), are called *translationengleiche* (or t-) subgroups because the set $\mathcal{T}$ of all (pure) translations is retained. In case (2), the point group $\mathcal{P}$ and thus the crystal class of the space group is unchanged. These subgroups are called *klassengleiche* or k-subgroups. In the general case (3), both the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ and the point group $\mathcal{P}$ are reduced; the subgroup has lost translations *and* belongs to a crystal class of lower order: these are *general* subgroups.

Obviously, the general subgroups are more difficult to survey than kinds (1) and (2). Fortunately, a theorem of Hermann (1929) states that if $\mathcal{H}$ is a proper subgroup of $\mathcal{G}$, then there always exists an intermediate group $\mathcal{M}$ such that $\mathcal{G} > \mathcal{M} > \mathcal{H}$, where $\mathcal{M}$ is a t-subgroup of $\mathcal{G}$ and $\mathcal{H}$ is a k-subgroup of $\mathcal{M}$. If $\mathcal{H} < \mathcal{G}$ is maximal, then either $\mathcal{M} = \mathcal{G}$ and $\mathcal{H}$ is a k-subgroup of $\mathcal{G}$ or $\mathcal{M} = \mathcal{H}$ and $\mathcal{H}$ is a t-subgroup of $\mathcal{G}$. It follows that a maximal subgroup of a space group $\mathcal{G}$ is either a t-subgroup or a k-subgroup of $\mathcal{G}$. According to this theorem, general subgroups can never occur among the maximal subgroups. They can, however, be derived by a stepwise process of linking maximal t-subgroups and maximal k-subgroups by the chains discussed above.

1.7.1.1. *Translationengleiche* (or t-) subgroups of space groups

The 'point group' $\mathcal{P}$ of a given space group $\mathcal{G}$ is a finite group, *cf.* Chapter 1.3. Hence, the number of subgroups and consequently the number of maximal subgroups of $\mathcal{P}$ is finite. There exist, therefore, only a finite number of maximal t-subgroups of $\mathcal{G}$. The possible t-subgroups were first listed in *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, Band 1 (1935); corrections have been reported by Ascher *et al.* (1969). All maximal t-subgroups are listed individually for each space group $\mathcal{G}$ in *IT* A1 with the index, the (unconventional) Hermann–Mauguin symbol referred to the coordinate system of $\mathcal{G}$, the space-group number and conventional Hermann–Mauguin symbol, their general position and the transformation to the conventional coordinate system of $\mathcal{H}$. This may involve a change of basis and an origin shift from the coordinate system of $\mathcal{G}$.

1.7.1.2. *Klassengleiche* (or *k*-) subgroups of space groups

Every space group $\mathcal{G}$ has an infinite number of maximal k-subgroups. For dimensions 1, 2 and 3, however, it can be shown that the number of maximal k-subgroups is finite if subgroups belonging to the same affine space-group type as $\mathcal{G}$ are excluded. The number of maximal subgroups of $\mathcal{G}$ belonging to the same affine space-group type as $\mathcal{G}$ is always infinite; these subgroups are called maximal *isomorphic* subgroups. Maximal *non-isomorphic klassengleiche* subgroups of plane groups and space groups always have index 2, 3 or 4. They are listed individually in *IT* A1 together with the isomorphic subgroups of the same index. For practical reasons, the k-subgroups are distributed into two lists headed 'Loss of centring translations' and 'Enlarged (conventional) unit cell'. The data consist of the index of the subgroup $\mathcal{H}$, the lattice relation between the lattices of $\mathcal{H}$ and $\mathcal{G}$, the characterization of the space group $\mathcal{H}$, the general position of $\mathcal{H}$ and the transformation from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$.

1.7.1.3. Isomorphic subgroups of space groups

The existence of isomorphic subgroups is of special interest. There can be no proper isomorphic subgroups $\mathcal{H} < \mathcal{G}$ of finite groups $\mathcal{G}$ because the difference of the orders $|\mathcal{H}| < |\mathcal{G}|$ does not allow isomorphism. The point group $\mathcal{P}$ of a space group $\mathcal{G}$ is finite and its order cannot be reduced if $\mathcal{H}$ is to be isomorphic to $\mathcal{G}$. Therefore, isomorphic subgroups are necessarily k-subgroups.

The number of isomorphic maximal subgroups and thus the number of all isomorphic subgroups of any space group is infinite. It can be shown that maximal subgroups of space groups of index $i > 4$ are necessarily isomorphic. Depending on the crystallographic equivalence of the coordinate axes, the index of the subgroup is p, p^2 or p^3, where p is a prime. The isomorphic subgroups cannot be listed individually because of their number, but they can be listed as members of a few series. The series are mostly determined by the index p; the members may be normal subgroups of $\mathcal{G}$ or they form conjugacy classes the size of which is either p, p^2 or p^3. The individual members of a conjugacy class are determined by the locations of their origins. The size of the conjugacy class, a basis for the lattice of the subgroup, the generators of the individual isomorphic subgroups and the coordinate transformation from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$ are listed in *IT* A1 for all space-group types.

Examples

Isomorphic subgroups of $P1$: the space group $P1$ is an abelian space group, all of its subgroups are isomorphic and are normal subgroups. The index may be any prime p.

Isomorphic subgroups of $P\bar{1}$: the space group $P\bar{1}$ is not abelian and subgroups exist of types $P1$ and $P\bar{1}$. The latter are isomorphic. Those of index 2 are normal subgroups; for higher index $p > 2$ they form conjugacy classes of prime size p.

Enantiomorphic space groups have an infinite number of maximal isomorphic subgroups of the same type and an infinite number of maximal isomorphic subgroups of the enantiomorphic type.

Example

All k-subgroups $\mathcal{H}$ of a given space group $\mathcal{G} = P3_1$ with basis vectors $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$, where p is any prime number other than 3, are maximal isomorphic subgroups. They belong to space-group type $P3_1$ if $p = 1 \bmod 3$. They belong to the enantiomorphic space-group type $P3_2$ if $p = 2 \bmod 3$.

In principle there is no difference in importance between t-, non-isomorphic k- and isomorphic k-subgroups. Roughly speaking, a group–subgroup relation is 'strong' if the index $[i]$ of the subgroup is low. All maximal t- and maximal non-isomorphic k-subgroups have indices less than four in $\mathbb{E}^2$ and less than five in $\mathbb{E}^3$, index four already being rather exceptional. Maximal isomorphic k-subgroups of arbitrarily high index exist for every space group.

1.7.1.4. Supergroups

Sometimes a space group $\mathcal{H}$ is known and the possible space groups $\mathcal{G}$, of which $\mathcal{H}$ is a subgroup, are of interest. A space group $\mathcal{R}$ is called a *minimal supergroup* of a space group $\mathcal{G}$ if $\mathcal{G}$ is a maximal subgroup of $\mathcal{R}$.

Examples of minimal supergroups

In Fig. 1.7.1.1, the space group $P6_3/mcm$ is a minimal supergroup of $P\bar{6}c2$, ..., $P\bar{3}c1$; $P\bar{6}c2$ is a minimal supergroup of $P\bar{6}$, $P3c1$ and $P312$; *etc*.

If $\mathcal{G}$ is a maximal t-subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal t-supergroup of $\mathcal{G}$. If $\mathcal{G}$ is a maximal k-subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal k-supergroup of $\mathcal{G}$. Finally, if $\mathcal{G}$ is a maximal isomorphic subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal isomorphic supergroup of $\mathcal{G}$. Data for minimal t- and minimal non-isomorphic k-supergroups are listed in *IT* A1, although in a less explicit way than that in which the subgroups are listed. The data essentially make the detailed subgroup data usable for the search for supergroups of space groups. Data on minimal isomorphic supergroups are not listed because they can be derived from the corresponding subgroup relations.

The search for supergroups $\mathcal{R} > \mathcal{G}$ of a space group $\mathcal{G}$ differs from the search for subgroups $\mathcal{H} < \mathcal{G}$ in one essential point: when looking for subgroups one knows the available group elements, namely the elements $g \in \mathcal{G}$; when looking for supergroups, any isometry $f \in \mathcal{E}$ may be a possible element of $\mathcal{R}$, $f \in \mathcal{R}$, where $\mathcal{E}$ is the Euclidean group of all isometries.

As we are mainly interested in the symmetries of crystal structures, it is reasonable only to look for groups $\mathcal{R}$ that are themselves space groups. In this way the search for supergroups of space groups is a reversal of the search for subgroups. Nevertheless, even then there are new phenomena; only two of these shall be mentioned here.

Example

For a given space group $P\bar{1}$, there is only one t-subgroup $P1$. However, for a space group $P1$, there is a continuously infinite number of t-supergroups $P\bar{1}$. Referred to the unit cell of $P1$, an additional centre of inversion can be placed in the range $0 \le x < \frac{1}{2}$, $0 \le y < \frac{1}{2}$, $0 \le z < \frac{1}{2}$. The centre in each of these locations leads to a new supergroup resulting in a continuous set of t-supergroups.

If $\mathcal{R}$ is a t-supergroup of $\mathcal{G}$ belonging to a crystal system with higher symmetry than that of $\mathcal{G}$, then the metric of $\mathcal{G}$ has to fulfil the conditions of the metric of $\mathcal{R}$. For example, if a tetragonal space group $\mathcal{G}$ has a cubic t-supergroup $\mathcal{R}$, then the lattice of $\mathcal{G}$ also has to have cubic symmetry.

In practice, small differences in the lattice parameters of $\mathcal{G}$ and $\mathcal{R}$ will occur, because lattice deviations can accompany a structural relationship.