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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 $P\bar{6}c2, \ldots, P\bar{3}c1$; $P\bar{6}c2$ 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.

  references