International Tables for Crystallography (2016). Vol. A, Section 1.7.1.1, p. 133.

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'.

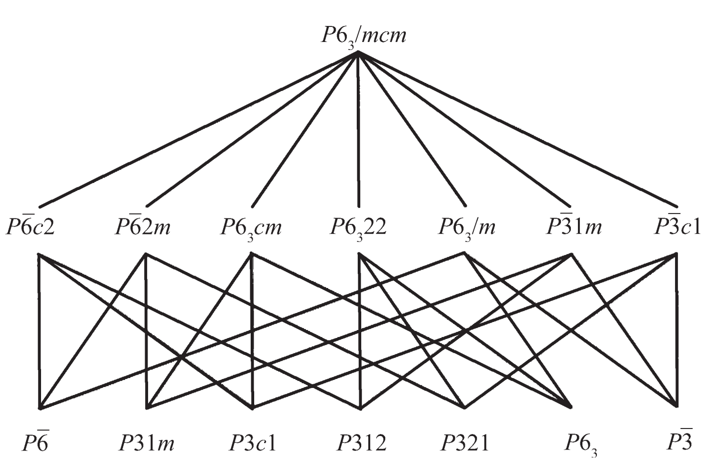

Figure 1.7.1.1
Space group $P6_3/mcm$ with *t*-subgroups of index 2 and 4. All 21 possible subgroup chains are displayed by lines.

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 $\mathcal{G}$.

references