International Tables for Crystallography (2006). Vol. A, Figure 8.3.3.1, p. 735.

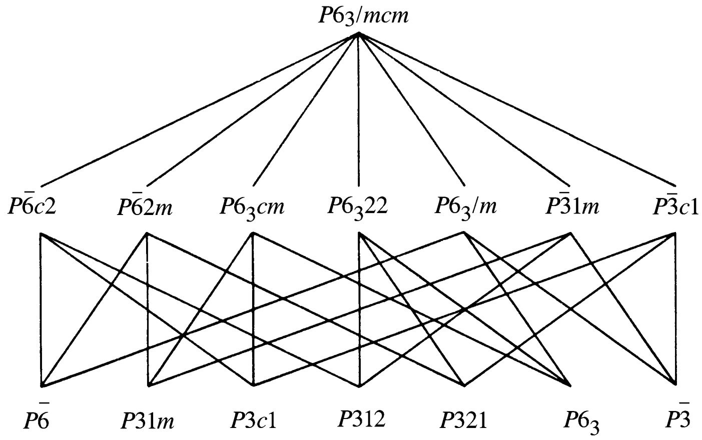

Fig. 8.3.3.1. Space group $P6_3/mcm$ with *t* subgroups of index [2] and [4]. All 21 possible subgroup chains are displayed by lines.

but eliminating all rotations and combinations of rotations with translations. For every space group of space-group type $P2$ such a subgroup $P1$ exists. Thus 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.

For every subgroup $\mathcal{H}$ of a space group $\mathcal{G}$, a 'right coset decomposition' of $\mathcal{G}$ relative to $\mathcal{H}$ can be defined as

$$\mathcal{G} = \mathcal{H} + \mathcal{H}\mathsf{G}_2 + \ldots + \mathcal{H}\mathsf{G}_i.$$

The elements $\mathsf{G}_2, \ldots, \mathsf{G}_i$ of $\mathcal{G}$ are such that G_j is contained only in the coset $\mathcal{H}\mathsf{G}_j$. The integer $[i]$, *i.e.* the number of cosets, is called the index of $\mathcal{H}$ in $\mathcal{G}$; *cf.* Section 8.1.6, footnote §.

The index $[i]$ of a subgroup has a geometric significance. It determines the 'dilution' of symmetry operations of $\mathcal{H}$ compared with those of $\mathcal{G}$. This dilution can occur in essentially three different ways:

(i) by reducing the order of the point group, *i.e.* by eliminating all symmetry operations of some kind. The example $P2 \rightarrow P1$ mentioned above is of this type.

(ii) 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 $(2u+1)\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, u, v, w integral (new basis $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$), and, hence, by eliminating half of the twofold axes, or

(*b*1) by $\mathbf{b}' = 2\mathbf{b}$, *i.e.* by thinning out the translations parallel to the twofold axes, or

(*b*2) again by $\mathbf{b}' = 2\mathbf{b}$ but replacing the twofold rotation axes by twofold screw axes.

(iii) by combination of (i) and (ii), *e.g.* by reducing the order of the point group *and* by thinning out the lattice of translations.

Subgroups of the first kind (i) are called *translationengleiche* or *t* subgroups* because the set $\mathcal{T}$ of all (pure) translations is retained. In case (ii), 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 (iii), both the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ and the point group $\mathcal{P}$ are changed; the subgroup has lost translations *and* belongs to a crystal class of lower order.

* Hermann (1929) used the term *zellengleich* but this term caused misunderstandings because it was sometimes understood to refer to the conventional unit cell. Not the conservation of the conventional unit cell but rather the retention of *all* translations of the space group is the essential feature of *t* subgroups.

Obviously the third kind (iii) of subgroups is more difficult to survey than kinds (i) and (ii). Fortunately, a theorem of Hermann states that the maximal subgroups of a space group $\mathcal{G}$ are of type (i) or (ii).

Theorem of Hermann (1929). 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, subgroups of kind (iii) can never occur among the maximal subgroups. They can, however, be derived by a stepwise process of linking maximal subgroups of types (i) and (ii), as has been shown by the chains discussed above.

8.3.3.1. *Translationengleiche or t subgroups of a space group*

The 'point group' $\mathcal{P}$ of a given space group $\mathcal{G}$ is a finite group. 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 $\mathcal{G}$. *All* maximal *t* subgroups of every space group $\mathcal{G}$ are listed in the space-group tables of this volume; *cf.* Section 2.2.15. The possible *t* subgroups were first listed by Hermann (1935); corrections have been reported by Ascher *et al.* (1969).

8.3.3.2. *Klassengleiche or k subgroups of a space group*

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*. In Part 13 isomorphic subgroups are treated in detail. In the space-group tables, only data on the isomorphic subgroups of lowest index are listed. The way in which the isomorphic and non-isomorphic *k* subgroups are listed in the space-group tables is described in Section 2.2.15.

Remark: 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 $\mathcal{G}'$ of a given space group $\mathcal{G} \equiv P3_1$, with basis vectors $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{b}, \mathbf{c}' = p\mathbf{c}, p$ being any prime number except 3, are maximal isomorphic subgroups. They belong to space-group type $P3_1$ if $p = 3r + 1, r$ any integer. They belong to the enantiomorphic space-group type $P3_2$ if $p = 3r + 2$.

Even though in the space-group tables some kinds of maximal subgroups are listed completely whereas others are listed only partly, it must be emphasized that 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 E^2 and five in E^3, index four already being rather exceptional. Maximal isomorphic *k* subgroups of arbitrarily high index exist for every space group.

8.3.3.3. *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.

Definition: A space group $\mathcal{R}$ is called a *minimal supergroup* of a space group $\mathcal{G}$ if $\mathcal{G}$ is a maximal subgroup of $\mathcal{R}$.