

## 8.3. SPECIAL TOPICS ON SPACE GROUPS

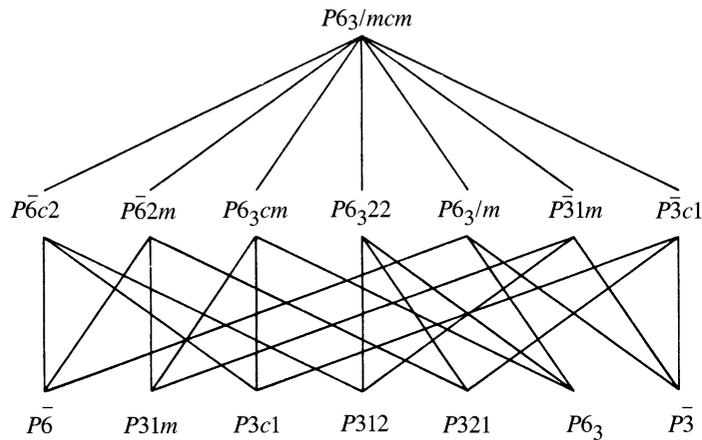


Fig. 8.3.3.1. Space group  $P6_3/mcm$  with  $t$  subgroups of index [2] and [4]. All 21 possible subgroup chains are displayed by lines.

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

$$\mathcal{G} = \mathcal{H} + \mathcal{H}G_2 + \dots + \mathcal{H}G_i.$$

The elements  $G_2, \dots, G_i$  of  $\mathcal{G}$  are such that  $G_j$  is contained only in the coset  $\mathcal{H}G_j$ . 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

(b1) by  $\mathbf{b}' = 2\mathbf{b}$ , i.e. by thinning out the translations parallel to the twofold axes, or

(b2) 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  $\mathcal{R}$ .