

## 3.2. POINT GROUPS AND CRYSTAL CLASSES

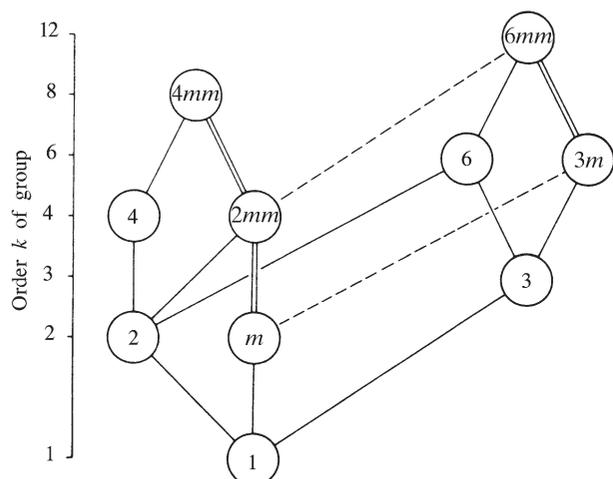


Figure 3.2.1.2

Maximal subgroups and minimal supergroups of the two-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left.

or rhombohedral: e.g. ‘hexagonal ogdohedry’ and ‘rhombohedral tetartohedry’.

## 3.2.1.3. Subgroups and supergroups of the crystallographic point groups

In this section, the sub- and supergroup relations between the crystallographic point groups are presented in the form of a ‘family tree’.<sup>12</sup> Figs. 3.2.1.2 and 3.2.1.3 apply to two and three dimensions. The sub- and supergroup relations between two groups are represented by solid or dashed lines. For a given point group  $\mathcal{P}$  of order  $k_{\mathcal{P}}$  the lines to groups of lower order connect  $\mathcal{P}$  with all its *maximal subgroups*  $\mathcal{H}$  with orders  $k_{\mathcal{H}}$ ; the index  $[i]$  of each subgroup is given by the ratio of the orders  $k_{\mathcal{P}}/k_{\mathcal{H}}$ . The lines to groups of higher order connect  $\mathcal{P}$  with all its *minimal supergroups*  $\mathcal{S}$  with orders  $k_{\mathcal{S}}$ ; the index  $[i]$  of each supergroup is given by the ratio  $k_{\mathcal{S}}/k_{\mathcal{P}}$ . In other words: if the diagram is read downwards, subgroup relations are displayed; if it is read upwards, supergroup relations are revealed. The index is always an integer (theorem of Lagrange) and can be easily obtained from the group orders given on the left of the diagrams. The highest index of a maximal subgroup is [3] for two dimensions and [4] for three dimensions.

Two important kinds of subgroups, namely sets of conjugate subgroups and normal subgroups, are distinguished by dashed and solid lines. They are characterized as follows:

The subgroups  $\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_n$  of a group  $\mathcal{P}$  are *conjugate subgroups* if  $\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_n$  are symmetry-equivalent in  $\mathcal{P}$ , i.e. if for every pair  $\mathcal{H}_i, \mathcal{H}_j$  at least one symmetry operation  $W$  of  $\mathcal{P}$  exists which maps  $\mathcal{H}_i$  onto  $\mathcal{H}_j$ :  $W^{-1}\mathcal{H}_iW = \mathcal{H}_j$ ; cf. Sections 1.1.5 and 1.1.8.

## Examples

- (1) Point group  $3m$  has three different mirror planes which are equivalent due to the threefold axis. In each of the three maximal subgroups of type  $m$ , one of these mirror planes is retained. Hence, the three subgroups  $m$  are conjugate in  $3m$ . This set of conjugate subgroups is represented by one dashed line in Figs. 3.2.1.2 and 3.2.1.3.

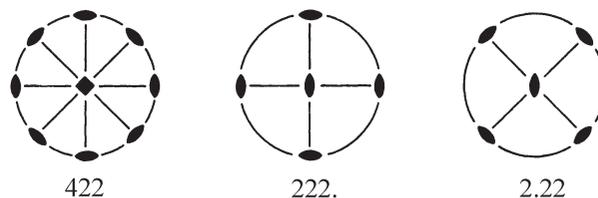
<sup>12</sup> This type of diagram was first used in *International Tables for the Determination of Crystal Structures* (1935); in *International Tables for X-ray Crystallography* (1952) a somewhat different approach was employed.

- (2) Similarly, group  $432$  has three maximal conjugate subgroups of type  $422$  and four maximal conjugate subgroups of type  $32$ .

The subgroup  $\mathcal{H}$  of a group  $\mathcal{P}$  is a *normal* (or invariant) subgroup if no subgroup  $\mathcal{H}'$  of  $\mathcal{P}$  exists that is conjugate to  $\mathcal{H}$  in  $\mathcal{P}$ . Note that this does not imply that  $\mathcal{H}$  is also a normal subgroup of any supergroup of  $\mathcal{P}$ . Subgroups of index [2] are always normal and maximal (cf. Section 1.1.5). (The role of normal subgroups for the structure of space groups is discussed in Sections 1.3.3 and 1.4.2.3.)

## Examples

- (1) Fig. 3.2.1.3 shows two solid lines between point groups  $422$  and  $222$ , indicating that  $422$  has two maximal normal subgroups  $222$  of index [2]. The symmetry elements of one subgroup are rotated by  $45^\circ$  around the  $c$  axis with respect to those of the other subgroup. Thus, in one subgroup the symmetry elements of the two secondary, in the other those of the two tertiary tetragonal symmetry directions (cf. Table 2.1.3.1) are retained, whereas the primary twofold axis is the same for both subgroups. There exists no symmetry operation of  $422$  that maps one subgroup onto the other. This is illustrated by the stereograms below. The two normal subgroups can be indicated by the ‘oriented symbols’  $222.$  and  $2.22$ .



- (2) Similarly, group  $432$  has one maximal normal subgroup,  $23$ .

Figs. 3.2.1.2 and 3.2.1.3 show that there exist two ‘summits’ in both two and three dimensions from which all other point groups can be derived by ‘chains’ of maximal subgroups. These summits are formed by the square and the hexagonal holohedry in two dimensions and by the cubic and the hexagonal holohedry in three dimensions.

The sub- and supergroups of the point groups are useful both in their own right and as a basis of the *translationengleiche* or *t* subgroups and supergroups of space groups (cf. Section 1.7.1). Tables of the sub- and supergroups of the plane groups and space groups are contained in Volume A1 of *International Tables for Crystallography* (2010). A general discussion of sub- and supergroups of crystallographic groups, together with further explanations and examples, is given in Section 1.7.1.

## 3.2.1.4. Noncrystallographic point groups

## 3.2.1.4.1. Description of general point groups

In Sections 3.2.1.2 and 3.2.1.3, only the 32 *crystallographic* point groups (crystal classes) are considered. In addition, infinitely many *noncrystallographic* point groups exist that are of interest as possible symmetries of molecules and of quasicrystals and as approximate local site symmetries in crystals. Crystallographic and noncrystallographic point groups are collected here under the name *general point groups*. They are reviewed in this section and listed in Tables 3.2.1.5 and 3.2.1.6.