

## 3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

names exist for 'isogonal' polyhedra. The maximal number of polyhedra required is three. The *shape* of the combination that describes the point form depends on the relative sizes of the polyhedra involved, *i.e.* on the relative values of their central distances. Moreover, in some cases even the *topology* of the point form may change.

*Example*

'Cube truncated by octahedron' and 'octahedron truncated by cube'. Both forms have 24 vertices, 14 faces and 36 edges, but the faces of the first combination are octagons and trigons, those of the second are hexagons and tetragons. These combinations represent different special point forms  $x, y, z$  and  $0, y, z$ . One form can change into the other only *via* the (semi-regular) cuboctahedron  $0, y, y$ , which has 12 vertices, 14 faces and 24 edges.

The unambiguous description of the cubic point forms by combinations of 'isohedral' polyhedra requires restrictions on the relative sizes of the polyhedra of a combination. The permissible range of the size ratios is limited on the one hand by vanishing, on the other hand by splitting of vertices of the combination. Three cases have to be distinguished:

(a) The relative sizes of the polyhedra of the combination can vary *independently*. This occurs whenever three edges meet in one vertex. In Table 3.2.3.2, the names of these point forms contain the term 'truncated'.

*Examples*

- (1) 'Octahedron truncated by cube' (24 vertices, dual to tetrahexahedron).
- (2) 'Cube truncated by two tetrahedra' (24 vertices, dual to hexatetrahedron), implying independent variation of the relative sizes of the two truncating tetrahedra.

(b) The relative sizes of the polyhedra are *interdependent*. This occurs for combinations of three polyhedra whenever four edges meet in one vertex. The names of these point forms contain the symbol '&'.

*Example*

'Cube & two tetrahedra' (12 vertices, dual to tetragon-tritetrahedron); here the interdependence results from the requirement that in the combination a cube edge is reduced to a vertex in which faces of the two tetrahedra meet. The location of this vertex on the cube edge is free. A higher-symmetry 'limiting' case of this combination is the 'cuboctahedron', where the two tetrahedra have the same sizes and thus form an octahedron.

(c) The relative sizes of the polyhedra are *fixed*. This occurs for combinations of three polyhedra if five edges meet in one vertex. These point forms are designated by special names (snub tetrahedron, snub cube, irregular icosahedron), or their names contain the symbol '+'. The cuboctahedron appears here too, as a limiting form of the snub tetrahedron (dual to pentagon-tritetrahedron) and of the irregular icosahedron (dual to pentagon-dodecahedron) for the special coordinates  $0, y, y$ .

(vi) Limiting crystal forms result from general or special crystal forms for special values of certain geometrical parameters of the form.

*Examples*

- (1) A pyramid degenerates into a prism if its apex angle becomes 0, *i.e.* if the apex moves towards infinity.
- (2) In point group 32, the general form is a trigonal trapezohedron  $\{hkl\}$ ; this form can be considered as two opposite trigonal pyramids, rotated with respect to each other by an angle  $\chi$ . The trapezohedron changes into the limiting forms 'trigonal dipyrmaid'  $\{hhl\}$  for  $\chi = 0^\circ$  and 'rhombohedral'  $\{h0l\}$  for  $\chi = 60^\circ$ .

(vii) One and the same type of polyhedron can occur as a general, special or limiting form.

*Examples*

- (1) A tetragonal dipyrmaid is a general form in point group  $4/m$ , a special form in point group  $4/mmm$  and a limiting general form in point groups  $422$  and  $\bar{4}2m$ .
- (2) A tetragonal prism appears in point group  $\bar{4}2m$  both as a basic special form (4b) and as a limiting special form (4c).

(viii) A peculiarity occurs for the cubic point groups. Here the crystal forms  $\{hhl\}$  are realized as two topologically different kinds of polyhedra with the same face symmetry, multiplicity and, in addition, the same eigensymmetry. The realization of one or other of these forms depends upon whether the Miller indices obey the conditions  $|h| > |l|$  or  $|h| < |l|$ , *i.e.* whether, in the stereographic projection, a face pole is located between the directions  $[110]$  and  $[111]$  or between the directions  $[111]$  and  $[001]$ . These two kinds of polyhedra have to be considered as two *realizations of one type* of crystal form because their face poles are located on the same set of conjugate symmetry elements. Similar considerations apply to the point forms  $x, x, z$ .

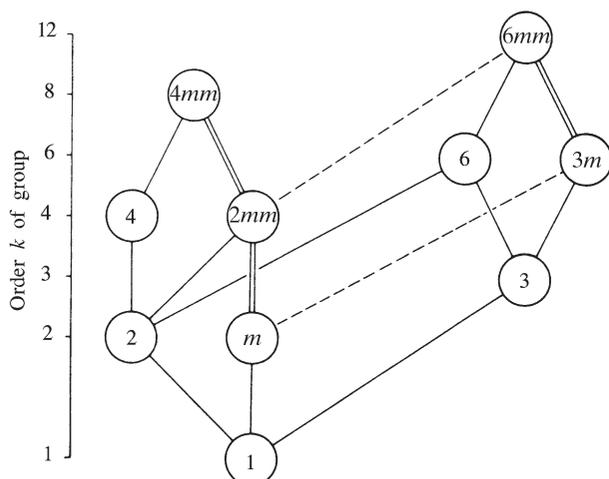
In the point groups  $m\bar{3}m$  and  $\bar{4}3m$ , the two kinds of polyhedra represent two realizations of one *special* 'Wyckoff position'; hence, they have the same Wyckoff letter. In the groups 23,  $m\bar{3}$  and 432, they represent two realizations of the same type of limiting *general* forms. In the tables of the cubic point groups, the two entries are always connected by braces.

The same kind of peculiarity occurs for the two icosahedral point groups, as mentioned in Section 3.2.1.4.2 and listed in Table 3.2.2.1.

## 3.2.1.2.5. Names and symbols of the crystal classes

Several different sets of names have been devised for the 32 crystal classes. Their use, however, has greatly declined since the introduction of the international point-group symbols. As examples, two sets (both translated into English) that are frequently found in the literature are given in Table 3.2.1.4. To the name of the class the name of the system has to be added: *e.g.* 'tetragonal pyramidal' or 'tetragonal tetartohedry'.

Note that Friedel (1926) based his nomenclature on the point symmetry of the lattice. Hence, two names are given for the five trigonal point groups, depending whether the lattice is hexagonal



**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  $k_P$  the lines to groups of lower order connect  $\mathcal{P}$  with all its *maximal subgroups*  $\mathcal{H}$  with orders  $k_H$ ; the index  $[i]$  of each subgroup is given by the ratio of the orders  $k_P/k_H$ . The lines to groups of higher order connect  $\mathcal{P}$  with all its *minimal supergroups*  $\mathcal{S}$  with orders  $k_S$ ; the index  $[i]$  of each supergroup is given by the ratio  $k_S/k_P$ . 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.

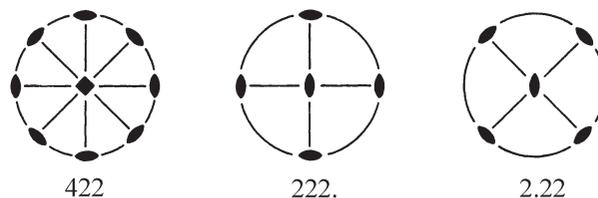
<sup>12</sup> This type of diagram was first used in *International Tables for the Determination of Crystal Structures* (1935); in *International Tables for X-ray Crystallography* (1952) a somewhat different approach was employed.

- (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.