# 3.2. Point groups and crystal classes

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## 3.2.1. Crystallographic and noncrystallographic point groups

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### 3.2.1.1. Introduction and definitions

A *point group*[1] is a group of symmetry operations all of which leave at least one point unmoved. Thus, all operations containing translations are excluded. Point groups can be subdivided into crystallographic and noncrystallographic point groups. A *crystallographic* point group is a point group that maps a point lattice onto itself. Consequently, rotations and rotoinversions are restricted to the well known crystallographic cases 1, 2, 3, 4, 6 and $\bar{1}$, $\bar{2} = m$, $\bar{3}$, $\bar{4}$, $\bar{6}$ (*cf.* Section 1.2.1); matrices for these symmetry operations are listed in Tables 1.2.2.1 and 1.2.2.2. No such restrictions apply to the *noncrystallographic* point groups.

The numbers of the crystallographic point groups are finite: 2 for one dimension, 10 for two dimensions and 32 for three dimensions. The numbers of noncrystallographic point groups for dimensions $n \geq 2$ are infinite. The two- and three-dimensional crystallographic point groups and their crystal systems are summarized in Tables 3.2.1.1 and 3.2.1.2. They are described in detail in Section 3.2.1.2. The two one-dimensional point groups are discussed in Section 2.1.3.16. The noncrystallographic point groups are treated in Section 3.2.1.4.

*Crystallographic* point groups occur:

(i) in vector space as symmetries of the external shapes of crystals, *i.e.* of the set of vectors normal to the crystal faces (morphological symmetry); this also includes the symmetries of sets of symmetry-equivalent net planes in crystals (reciprocal-lattice points), fundamental for the theory of X-ray diffraction.

(ii) in point space as site symmetries of points in lattices or in crystal structures and as symmetries of molecules, atomic groups and coordination polyhedra.

*General* point groups, *i.e.* crystallographic *and* noncrystallographic point groups, occur as:

(iii) symmetries of (rigid) molecules (molecular symmetry):

(iv) symmetries of physical properties of crystals (*e.g.* tensor symmetries); here noncrystallographic point groups with axes of order infinity are of particular importance, as in the symmetries of circles, spheres or rotation ellipsoids:

(v) approximate symmetries of the local environment of a point in a crystal structure, *i.e.* as *local* site symmetries. Examples are sphere-like atoms or ions in crystals, as well as icosahedral atomic groups. These noncrystallographic symmetries, however, are only approximate, even for the close neighbourhood of a site.

A (geometric) *crystal class* (point-group type) is the set of all crystals having the same point-group symmetry. The word 'class', therefore, denotes a classificatory pigeonhole and should not be used as synonymous with the point group of a particular crystal. The symbol of a crystal class is that of the common point group. (For geometric and arithmetic crystal classes of space groups, see Sections 1.3.4.2 and 1.3.4.4.)

Of particular importance for the structure determination of crystals are the 11 *centrosymmetric crystallographic point groups*, because they describe the possible symmetries of the diffraction record of a crystal: $\bar{1}$; $2/m$; $mmm$; $4/m$; $4/mmm$; $\bar{3}$; $\bar{3}m$; $6/m$; $6/mmm$; $m\bar{3}$; $m\bar{3}m$. This is due to Friedel's rule, which states that, provided anomalous dispersion is neglected, the diffraction record of any crystal is centrosymmetric, even if the crystal is noncentrosymmetric. The symmetry of the diffraction record determines the *Laue class* of the crystal; this is further explained in Chapter 1.6. For a given crystal, its Laue class is obtained if a symmetry centre is added to its point group, as shown in Table 3.2.2.1.

In two dimensions, six 'centrosymmetric' crystallographic point groups and hence six two-dimensional Laue classes exist: 2; 2*mm*; 4; 4*mm*; 6; 6*mm*. These point groups are, for instance, the only possible symmetries of zero-layer X-ray photographs.

Among the centrosymmetric crystallographic point groups in three dimensions, the seven *lattice point groups* (holohedral point groups, *holohedries*) are of special importance because they constitute the possible point symmetries of lattices, *i.e.* the site symmetries of their nodes. In three dimensions, the seven holohedries are: $\bar{1}$; $2/m$; $mmm$; $4/mmm$; $\bar{3}m$; $6/mmm$; $m\bar{3}m$. Note that $\bar{3}m$ is the point symmetry of the rhombohedral lattice and $6/mmm$ the point symmetry of the hexagonal lattice; both occur in the hexagonal crystal family (*cf.* Chapter 2.1). Point groups that are, within a crystal family, subgroups of a holohedry are called merohedries; they are called specifically hemihedries for subgroups of index 2, tetartohedries for index 4 and ogdohedries for index 8.

In two dimensions, four holohedries exist: 2; 2*mm*; 4*mm*; 6*mm*. Note that the hexagonal crystal family in two dimensions contains only one lattice type, with point symmetry 6*mm*.

Another classification of the crystallographic point groups is that into isomorphism classes. Here all those point groups that have the same kind of group table appear in one class. These isomorphism classes are also known under the name of *abstract point groups*.

There are 18 abstract crystallographic point groups in three dimensions: the point groups in each of the following lines are isomorphous and belong to the same abstract group:

**Table 3.2.1.1**
The ten two-dimensional crystallographic point groups, arranged according to crystal system

The dashed line separates point groups with different Laue classes within one crystal system.

| General symbol | Crystal system | | | | |
|---|---|---|---|---|---|
| | Oblique (top) Rectangular (bottom) | | Square | Hexagonal | |
| $n$ | 1 | 2 | 4 | 3 | 6 |
| $nmm$ | $m$ | 2*mm* | 4*mm* | 3*m* | 6*mm* |

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[1] For reasons of simplicity, in this chapter the same term 'point group' is used for a 'particular point group' *and* a 'type of point group'. For space groups, this distinction is explained in Section 1.3.4.1. For a different use of the term 'point group' see Section 1.3.3.1.

**Table 3.2.1.2**

The 32 three-dimensional crystallographic point groups, arranged according to crystal system (*cf.* Chapter 2.1)

Full Hermann–Mauguin (left) and Schoenflies symbols (right). The dashed line separates point groups with different Laue classes within one crystal system. A brief introduction to point-group symbols is provided in Hahn & Klapper (2005).

| General symbol | Crystal system | | | | | | |
| | Triclinic | Monoclinic (top) Orthorhombic (bottom) | | Tetragonal | | Trigonal | |
|---|---|---|---|---|---|---|---|
| $n$ | 1 $C_1$ | 2 | $C_2$ | 4 | $C_4$ | 3 | $C_3$ |
| $\bar{n}$ | $\bar{1}$ $C_i$ | $m \equiv \bar{2}$ | $C_s$ | $\bar{4}$ | $S_4$ | $\bar{3}$ | $C_{3i}$ |
| $n/m$ | | $2/m$ | $C_{2h}$ | $4/m$ | $C_{4h}$ | – | – |
| $n22$ | | 222 | $D_2$ | 422 | $D_4$ | 32 | $D_3$ |
| $nmm$ | | $mm2$ | $C_{2v}$ | $4mm$ | $C_{4v}$ | $3m$ | $C_{3v}$ |
| $\bar{n}2m$ | | – | – | $\bar{4}2m$ | $D_{2d}$ | $\bar{3}2/m$ | $D_{3d}$ |
| $n/m\,2/m\,2/m$ | | $2/m\,2/m\,2/m$ | $D_{2h}$ | $4/m\,2/m\,2/m$ | $D_{4h}$ | – | – |

| Hexagonal | | Cubic | |
|---|---|---|---|
| 6 | $C_6$ | 23 | $T$ |
| $\bar{6} \equiv 3/m$ | $C_{3h}$ | – | – |
| $6/m$ | $C_{6h}$ | $2/m\bar{3}$ | $T_h$ |
| 622 | $D_6$ | 432 | $O$ |
| $6mm$ | $C_{6v}$ | – | – |
| $\bar{6}2m$ | $D_{3h}$ | $\bar{4}3m$ | $T_d$ |
| $6/m\,2/m\,2/m$ | $D_{6h}$ | $4/m\,\bar{3}\,2/m$ | $O_h$ |

Order 1: 1
2: $\bar{1}$, 2, $m$
3: 3
4: $2/m$, 222, $mm2$
4: 4, $\bar{4}$
6: $\bar{3}$, 6, $\bar{6}$
6: 32, $3m$
8: $mmm$
8: $4/m$

Order 8: 422, $4mm$, $\bar{4}2m$
12: $6/m$
12: $\bar{3}m$, 622, $6mm$, $\bar{6}2m$
12: 23
16: $4/mmm$
24: $6/mmm$
24: $m\bar{3}$
24: 432, $\bar{4}3m$
48: $m\bar{3}m$.

In two dimensions, the ten crystallographic point groups form nine abstract groups; the groups 2 and *m* are isomorphous and belong to the same abstract group, the remaining eight point groups correspond to one abstract group each.

### 3.2.1.2. Crystallographic point groups

#### 3.2.1.2.1. Description of point groups

In crystallography, point groups usually are described

(i) by means of their Hermann–Mauguin or Schoenflies symbols;

(ii) by means of their stereographic projections;

(iii) by means of the matrix representations of their symmetry operations, frequently listed in the form of Miller indices (*hkl*) of the equivalent general crystal faces;

(iv) by means of drawings of actual crystals, natural or synthetic.

Descriptions (i) through (iii) are given in this section, whereas for crystal drawings and actual photographs reference is made to textbooks of crystallography and mineralogy [Buerger (1956, ch. 10) and Phillips (1971, chs. 3, 4 and 6) are particularly rich in pictures of crystal morphologies]; this also applies to the construction and the properties of the stereographic projection.

In Tables 3.2.3.1 and 3.2.3.2, the two- and three-dimensional crystallographic point groups are listed and described. The tables are arranged according to crystal systems and Laue classes. Within each crystal system and Laue class, the sequence of the point groups corresponds to that in the space-group tables of this volume: pure rotation groups are followed by groups containing reflections, rotoinversions and inversions. The holohedral point group is always given last.

In Tables 3.2.3.1 and 3.2.3.2, some point groups are described in *two or three versions*, in order to bring out the relations to the corresponding space groups (*cf.* Section 2.1.3.2):

(*a*) The three monoclinic point groups 2, *m* and $2/m$ are given with two settings, one with 'unique axis *b*' and one with 'unique axis *c*'.

(*b*) The two point groups $\bar{4}2m$ and $\bar{6}m2$ are described for two orientations with respect to the crystal axes, as $\bar{4}2m$ and $\bar{4}m2$ and as $\bar{6}m2$ and $\bar{6}2m$.

(*c*) The five trigonal point groups 3, $\bar{3}$, 32, $3m$ and $\bar{3}m$ are treated with two axial systems, 'hexagonal axes' and 'rhombohedral axes'.

(*d*) The hexagonal-axes description of the three trigonal point groups 32, $3m$ and $\bar{3}m$ is given for two orientations, as 321 and 312, as $3m1$ and $31m$, and as $\bar{3}m1$ and $\bar{3}1m$; this applies also to the two-dimensional point group $3m$.

The presentation of the point groups is similar to that of the space groups in Part 2. The *headline* contains the short Hermann–Mauguin and the Schoenflies symbols. The full Hermann–Mauguin symbol, if different, is given below the short symbol. No Schoenflies symbols exist for two-dimensional groups. For an explanation of the symbols see Sections 1.4.1 and 2.1.3.4, and Chapter 3.3.

Next to the headline, a pair of *stereographic projections* is given. The diagram on the left displays a general crystal or point form, that on the right shows the 'framework of symmetry elements'. Except as noted below, the *c* axis is always normal to the plane of the figure, the *a* axis points down the page and the *b* axis runs horizontally from left to right. For the five trigonal point groups, the *c* axis is normal to the page only for the description with 'hexagonal axes'; if described with 'rhombohedral axes', the direction [111] is normal and the positive *a* axis slopes towards the observer. The conventional coordinate systems used for the various crystal systems are listed in Table 2.1.1.1 and illustrated in Figs. 2.1.3.1 to 2.1.3.10.

In the *right-hand projection*, the graphical symbols of the symmetry elements are the same as those used in the space-group diagrams; they are listed in Chapter 2.1. Note that the symbol of a symmetry centre, a small circle, is also used for a face pole in the left-hand diagram. Mirror planes are indicated by heavy solid lines or circles; thin lines are used for the projection circle, for symmetry axes in the plane and for some special zones in the cubic system.

In the *left-hand projection*, the projection circle and the coordinate axes are indicated by thin solid lines, as are again some special zones in the cubic system. The dots and circles in this projection can be interpreted in two ways.

(i) As *general face poles*, where they represent general crystal faces which form a polyhedron, the 'general crystal form' (face form) {*hkl*} of the point group (see below). In two dimensions, edges, edge poles, edge forms and polygons take the place of faces, face poles, crystal forms (face forms) and polyhedra in three dimensions.

Face poles marked as dots lie above the projection plane and represent faces which intersect the positive $c$ axis[2] (positive Miller index $l$), those marked as circles lie below the projection plane (negative Miller index $l$). In two dimensions, edge poles always lie on the pole circle.

(ii) As *general points* (centres of atoms) that span a polyhedron or polygon, the 'general crystallographic point form' $x, y, z$. This interpretation is of interest in the study of coordination polyhedra, atomic groups and molecular shapes. The polyhedron or polygon of a point form is dual to the polyhedron of the corresponding crystal form.[3]

The general, special and limiting *crystal forms* and *point forms* constitute the main part of the table for each point group. The theoretical background is given below in Section 3.2.1.2.2, *Crystal and point forms* and an explanation of the listed data is to be found in Section 3.2.1.2.3, *Description of crystal and point forms.*

The last entry for each point group contains the *Symmetry of special projections*, *i.e.* the plane point group that is obtained if the three-dimensional point group is projected along a symmetry direction. The special projection directions are the same as for the space groups; they are listed in Section 2.1.3.14. The relations between the axes of the three-dimensional point group and those of its two-dimensional projections can easily be derived with the help of the stereographic projection. No projection symmetries are listed for the two-dimensional point groups.

Note that the symmetry of a projection along a certain direction may be higher than the symmetry of the crystal face normal to that direction. For example, in point group $\bar{1}$ all faces have face symmetry 1, whereas projections along any direction have symmetry 2; in point group 422, the faces (001) and (00$\bar{1}$) have face symmetry 4, whereas the projection along [001] has symmetry $4mm$.

### 3.2.1.2.2. Crystal and point forms

For a point group $\mathcal{P}$ a *crystal form* is a set of all symmetry-equivalent faces; a *point form* is a set of all symmetry-equivalent points. Crystal and point forms in point groups correspond to 'crystallographic orbits' in space groups; *cf.* Sections 1.1.7 and 1.4.4.1.

Two kinds of crystal and point forms with respect to $\mathcal{P}$ can be distinguished. They are defined as follows:

(i) *General form*: A *face* is called 'general' if only the identity operation transforms the face onto itself. Each complete set of symmetry-equivalent 'general faces' is a *general crystal form*. The *multiplicity* of a general form, *i.e.* the number of its faces, is the order of $\mathcal{P}$. In the stereographic projection, the poles of general faces do *not* lie on symmetry elements of $\mathcal{P}$.

A *point* is called 'general' if its *site symmetry*, *i.e.* the group of symmetry operations that transforms this point onto itself, is 1. A *general point form* is a complete set of symmetry-equivalent 'general points'.

(ii) *Special form*: A *face* is called 'special' if it is transformed onto itself by at least one symmetry operation of $\mathcal{P}$, in addition to the identity. Each complete set of symmetry-equivalent 'special faces' is called a *special crystal form*. The *face symmetry* of a special face is the group of symmetry operations that transforms this face onto itself; it is a subgroup of $\mathcal{P}$. The multiplicity of a special crystal form is the multiplicity of the general form divided by the order of the face-

symmetry group. In the stereographic projection, the poles of special faces lie on symmetry elements of $\mathcal{P}$. The Miller indices of a special crystal form obey restrictions like {$hk0$}, {$hhl$}, {100}.

A *point* is called 'special' if its *site symmetry* is higher than 1. A special point form is a complete set of symmetry-equivalent 'special points'. The multiplicity of a special point form is the multiplicity of the general form divided by the order of the site-symmetry group. It is thus the same as that of the corresponding special crystal form. The coordinates of the points of a special point form obey restrictions, like $x, y, 0$; $x, x, z$; $x, 0, 0$.

In two dimensions, point groups 1, 2, 3, 4 and 6 and, in three dimensions, point groups 1 and $\bar{1}$ have no special crystal forms.

General and special crystal and point forms can be represented by their sets of equivalent Miller indices {$hkl$} and point coordinates $x, y, z$. Each set of these 'triplets' stands for infinitely many crystal forms or point forms which are obtained by independent variation of the values and signs of the Miller indices $h, k, l$ or the point coordinates $x, y, z$.

It should be noted that for crystal forms, owing to the well known 'law of rational indices', the indices $h, k, l$ must be integers; no such restrictions apply to the coordinates $x, y, z$, which can be rational or irrational numbers.

*Example*

In point group 4, the general crystal form {$hkl$} stands for the set of all possible tetragonal pyramids, pointing either upwards or downwards, depending on the sign of $l$; similarly, the general point form $x, y, z$ includes all possible squares, lying either above or below the origin, depending on the sign of $z$. For the limiting cases $l = 0$ or $z = 0$, see below.

In order to survey the infinite number of possible forms of a point group, they are classified into *Wyckoff positions of crystal and point forms,* for short *Wyckoff positions*. This name has been chosen in analogy to the Wyckoff positions of space groups; *cf.* Sections 1.4.4.2 and 2.1.3.11. In point groups, the term 'position' can be visualized as the position of the face poles and points in the stereographic projection. Each 'Wyckoff position' is labelled by a *Wyckoff letter*.

*Definition*

A 'Wyckoff position of crystal and point forms' consists of all those crystal forms (point forms) of a point group $\mathcal{P}$ for which the face poles (points) are positioned on the same set of conjugate symmetry elements of $\mathcal{P}$; *i.e.* for each face (point) of one form there is one face (point) of every other form of the same 'Wyckoff position' that has exactly the same face (site) symmetry.

Each point group contains one 'general Wyckoff position' comprising all *general* crystal and point forms. In addition, up to two 'special Wyckoff positions' may occur in two dimensions and up to six in three dimensions. They are characterized by the different sets of conjugate face and site symmetries and correspond to the seven positions of a pole in the interior, on the three edges, and at the three vertices of the so-called 'characteristic triangle' of the stereographic projection.

*Examples*

(1) All tetragonal pyramids {$hkl$} and tetragonal prisms {$hk0$} in point group 4 have face symmetry 1 and belong to the same general 'Wyckoff position' 4$b$, with Wyckoff letter $b$.

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[2] This does not apply to 'rhombohedral axes': here the positive directions of all three axes slope upwards from the plane of the paper: *cf.* Fig. 2.1.3.9.
[3] Dual polyhedra have the same number of edges, but the numbers of faces and vertices are interchanged; *cf.* textbooks of geometry.

(2) All tetragonal pyramids *and* tetragonal prisms in point group 4*mm* belong to two special 'Wyckoff positions', depending on the orientation of their face-symmetry groups *m* with respect to the crystal axes: For the 'oriented face symmetry' *.m.*, the forms {*h0l*} and {100} belong to Wyckoff position 4*c*; for the oriented face symmetry *..m*, the forms {*hhl*} and {110} belong to Wyckoff position 4*b*. The face symmetries *.m.* and *..m* are not conjugate in point group 4*mm*. For the analogous 'oriented site symmetries' in space groups, see Section 2.1.3.12.

It is instructive to subdivide the crystal forms (point forms) of one Wyckoff position further, into *characteristic* and *noncharacteristic* forms. For this, one has to consider two symmetries that are connected with each crystal (point) form:

 (i) the point group $\mathcal{P}$ by which a form is generated (*generating point group*), *i.e.* the point group in which it occurs;
(ii) the full symmetry (inherent symmetry) of a form (considered as a polyhedron by itself), here called eigensymmetry $\mathcal{E}$. The *eigensymmetry point group* $\mathcal{E}$ is either the generating point group itself or a supergroup of it.

*Examples*
 (1) Each tetragonal pyramid {*hkl*} ($l \neq 0$) of Wyckoff position 4*b* in point group 4 has generating symmetry 4 and eigensymmetry 4*mm*; each tetragonal prism {*hk*0} of the same Wyckoff position has generating symmetry 4 again, but eigensymmetry 4/*mmm*.
 (2) A cube {100} may have generating symmetry 23, $m\overline{3}$, 432, $\overline{4}3m$ or $m\overline{3}m$, but its eigensymmetry is always $m\overline{3}m$.

The eigensymmetries and the generating symmetries of the 47 crystal forms (point forms) are listed in Table 3.2.1.3. With the help of this table, one can find the various point groups in which a given crystal form (point form) occurs, as well as the face (site) symmetries that it exhibits in these point groups; for experimental methods see Sections 3.2.2.2 and 3.2.2.3. Diagrams of the 47 crystal forms are presented in Fig. 3.2.1.1.

With the help of the two groups $\mathcal{P}$ and $\mathcal{E}$, each crystal or point form occurring in a particular point group can be assigned to one of the following two categories:

 (i) *characteristic* form, if eigensymmetry $\mathcal{E}$ and generating symmetry $\mathcal{P}$ are the same;
(ii) *noncharacteristic* form, if $\mathcal{E}$ is a proper supergroup of $\mathcal{P}$.

The importance of this classification will be apparent from the following examples.

*Examples*
 (1) A pedion and a pinacoid are noncharacteristic forms in all crystallographic point groups in which they occur:
 (2) all other crystal or point forms occur as characteristic forms in their eigensymmetry group $\mathcal{E}$;
 (3) a tetragonal pyramid is noncharacteristic in point group 4 and characteristic in 4*mm*;
 (4) a hexagonal prism can occur in nine point groups (12 Wyckoff positions) as a noncharacteristic form; in 6/*mmm*, it occurs in two Wyckoff positions as a characteristic form.

The general forms of the 13 point groups with no, or only one, symmetry direction ('monoaxial groups') 1, 2, 3, 4, 6, $\overline{1}$, *m*, $\overline{3}$, $\overline{4}$, $\overline{6} = 3/m, 2/m, 4/m, 6/m$ are always noncharacteristic, *i.e.* their eigensymmetries are enhanced in comparison with the generating point groups. The general positions of the other 19 point groups always contain characteristic crystal forms that may be used to

determine the point group of a crystal uniquely (*cf.* Section 3.2.2).[4]

So far, we have considered the occurrence of one crystal or point form in different point groups and different Wyckoff positions. We now turn to the occurrence of different kinds of crystal or point forms in one and the same Wyckoff position of a particular point group.

In a Wyckoff position, crystal forms (point forms) of different eigensymmetries may occur; the crystal forms (point forms) with the lowest eigensymmetry (which is always well defined) are called *basic forms* (German: *Grundformen*) of that Wyckoff position. The crystal and point forms of higher eigensymmetry are called *limiting forms* (German: *Grenzformen*) (*cf.* Table 3.2.1.3). These forms are always noncharacteristic.

Limiting forms[5] occur for certain restricted values of the Miller indices or point coordinates. They always have the same multiplicity and oriented face (site) symmetry as the corresponding basic forms because they belong to the same Wyckoff position. The enhanced eigensymmetry of a limiting form may or may not be accompanied by a change in the topology[6] of its polyhedra, compared with that of a basic form. In every case, however, the name of a limiting form is different from that of a basic form.

The face poles (or points) of a limiting form lie on symmetry elements of a supergroup of the point group that are not symmetry elements of the point group itself. There may be several such supergroups.

*Examples*
 (1) In point group 4, the (noncharacteristic) crystal forms {*hkl*} ($l \neq 0$) (tetragonal pyramids) of eigensymmetry 4*mm* are basic forms of the general Wyckoff position 4*b*, whereas the forms {*hk*0} (tetragonal prisms) of higher eigensymmetry 4/*mmm* are 'limiting general forms'. The face poles of forms {*hk*0} lie on the horizontal mirror plane of the supergroup 4/*m*.
 (2) In point group 4*mm*, the (characteristic) special crystal forms {*h0l*} with eigensymmetry 4*mm* are 'basic forms' of the special Wyckoff position 4*c*, whereas {100} with eigensymmetry 4/*mmm* is a 'limiting special form'. The face poles of {100} are located on the intersections of the vertical mirror planes of the point group 4*mm* with the horizontal mirror plane of the supergroup 4/*mmm*, *i.e.* on twofold axes of 4/*mmm*.

Whereas basic and limiting forms belonging to one 'Wyckoff position' are always clearly distinguished, closer inspection shows that a Wyckoff position may contain different 'types' of limiting forms. We need, therefore, a further criterion to classify the limiting forms of one Wyckoff position into types: A *type of limiting form of a Wyckoff position* consists of all those limiting forms for which the face poles (points) are located on the same set of additional conjugate symmetry elements of the holohedral point group (for the trigonal point groups, the hexagonal holo-

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[4] For a survey of these relations, as well as of the 'limiting forms', it is helpful to consider the (seven) *normalizers* of the crystallographic point groups in the group of all rotations and reflections (orthogonal group, sphere group); normalizers of the crystallographic and noncrystallographic point groups are listed in Tables 3.5.4.1 and 3.5.4.2.
[5] The treatment of 'limiting forms' in the literature is quite ambiguous. In some textbooks, limiting forms are omitted or treated as special forms in their own right: other authors define only limiting *general* forms and consider limiting *special* forms as if they were new special forms. For additional reading, see P. Niggli (1941, pp. 80–98).
[6] The topology of a polyhedron is determined by the numbers of its vertices, edges and faces, by the number of vertices of each face and by the number of faces meeting in each vertex.

**Table 3.2.1.3**

The 47 crystallographic face and point forms, their names, eigensymmetries, and their occurrence in the crystallographic point groups (generating point groups)

The oriented face (site) symmetries of the forms are given in parentheses after the Hermann–Mauguin symbol (column 6); a symbol such as $mm2(.m., m..)$ indicates that the form occurs in point group $mm2$ twice, with face (site) symmetries $.m.$ and $m..$. Basic (general and special) forms are printed in bold face, limiting (general and special) forms in normal type. The various settings of point groups $32$, $3m$, $\bar{3}m$, $\bar{4}2m$ and $\bar{6}2m$ are connected by braces. The 47 crystal forms are shown in Fig. 3.2.1.1. (Note that the numbering of the forms in column 1 does not correspond to the numbering used in Fig. 3.2.1.1.)

| No. | Crystal form | Point form | Number of faces or points | Eigensymmetry | Generating point groups with oriented face (site) symmetries between parentheses |
|---|---|---|---|---|---|
| 1 | Pedion or monohedron | Single point | 1 | $\infty m$ | $\mathbf{1(1)};\ \mathbf{2(2)};\ \boldsymbol{m(m)};\ \mathbf{3(3)};\ \mathbf{4(4)};$ $\mathbf{6(6)};\ \mathbf{mm2(mm2)};\ \mathbf{4mm(4mm)};$ $\mathbf{3m(3m)};\ \mathbf{6mm(6mm)}$ |
| 2 | Pinacoid or parallelohedron | Line segment through origin | 2 | $\dfrac{\infty}{m}m$ | $\mathbf{\bar{1}(1)};\ 2(1);\ m(1);\ \dfrac{\mathbf{2}}{\boldsymbol{m}}\mathbf{(2, m)};\ \mathbf{222(2.., .2., ..2)};$ $\mathbf{mm2}(.m., m..);\ \mathbf{mmm(2mm, m2m, mm2)};$ $\mathbf{\bar{4}}(2..);\ \dfrac{\mathbf{4}}{\boldsymbol{m}}(4..);\ 422(4..);\ \left\{\begin{array}{l}\mathbf{\bar{4}2m}(2.mm)\\ \mathbf{\bar{4}m2}(2mm.)\end{array}\right.;$ $\dfrac{\mathbf{4}}{\boldsymbol{m}}\mathbf{mm(4mm)};\ \bar{3}(3);\ \left\{\begin{array}{l}321(3..)\\312(3..)\\32\ \ (3.)\end{array}\right.;\ \left\{\begin{array}{l}\mathbf{\bar{3}m1}(3m.)\\ \mathbf{\bar{3}1m}(3.m)\\ \mathbf{\bar{3}m}\ \ (3m)\end{array}\right.;$ $\bar{6}(3..);\ \dfrac{\mathbf{6}}{\boldsymbol{m}}(6..);\ 622(6..);$ $\left\{\begin{array}{l}\mathbf{\bar{6}m2}(3m.)\\ \mathbf{\bar{6}2m}(3.m)\end{array}\right.;\ \dfrac{\mathbf{6}}{\boldsymbol{m}}\mathbf{mm(6mm)}$ |
| 3 | Sphenoid, dome, or dihedron | Line segment | 2 | $mm2$ | $\mathbf{2(1)};\ \boldsymbol{m(1)};\ \mathbf{mm2}(.m., m..)$ |
| 4 | Rhombic disphenoid or rhombic tetrahedron | Rhombic tetrahedron | 4 | 222 | $\mathbf{222(1)}$ |
| 5 | Rhombic pyramid | Rectangle | 4 | $mm2$ | $\mathbf{mm2(1)}$ |
| 6 | Rhombic prism | Rectangle through origin | 4 | $mmm$ | $\mathbf{2/m(1)};\ 222(1)\dagger;\ mm2(1);\ \mathbf{mmm}(m.., .m., ..m)$ |
| 7 | Rhombic dipyramid | Rectangular prism | 8 | $mmm$ | $\mathbf{mmm(1)}$ |
| 8 | Tetragonal pyramid | Square | 4 | $4mm$ | $\mathbf{4(1)};\ \mathbf{4mm}(..m, .m.)$ |
| 9 | Tetragonal disphenoid or tetragonal tetrahedron | Tetragonal tetrahedron | 4 | $\bar{4}2m$ | $\mathbf{\bar{4}(1)};\ \left\{\begin{array}{l}\mathbf{\bar{4}2m}(..m)\\ \mathbf{\bar{4}m2}(.m.)\end{array}\right.$ |
| 10 | Tetragonal prism | Square through origin | 4 | $\dfrac{4}{m}mm$ | $4(1);\ \bar{4}(1);\ \dfrac{\mathbf{4}}{\boldsymbol{m}}(m..);\ \mathbf{422}(..2, .2.);\ 4mm(..m, .m.);$ $\ddagger\left\{\begin{array}{l}\bar{4}2m(.2.)\ \text{and}\ \bar{4}2m(..m)\\ \bar{4}m2(..2)\ \text{and}\ \bar{4}m2(.m.)\end{array}\right.;$ $\dfrac{\mathbf{4}}{\boldsymbol{m}}\mathbf{mm}(m.m2, m2m.)$ |
| 11 | Tetragonal trapezohedron | Twisted tetragonal antiprism | 8 | 422 | $\mathbf{422(1)}$ |
| 12 | Ditetragonal pyramid | Truncated square | 8 | $4mm$ | $\mathbf{4mm(1)}$ |
| 13 | Tetragonal scalenohedron | Tetragonal tetrahedron cut off by pinacoid | 8 | $\bar{4}2m$ | $\left\{\begin{array}{l}\mathbf{\bar{4}2m(1)}\\ \mathbf{\bar{4}m2(1)}\end{array}\right.$ |
| 14 | Tetragonal dipyramid | Tetragonal prism | 8 | $\dfrac{4}{m}mm$ | $\dfrac{\mathbf{4}}{\boldsymbol{m}}\mathbf{(1)};\ 422(1)\dagger;\ \left\{\begin{array}{l}\bar{4}2m(1)\\ \bar{4}m2(1)\end{array}\right.;\ \dfrac{\mathbf{4}}{\boldsymbol{m}}\mathbf{mm}(.m, .m.)$ |
| 15 | Ditetragonal prism | Truncated square through origin | 8 | $\dfrac{4}{m}mm$ | $422(1);\ 4mm(1);\ \left\{\begin{array}{l}\bar{4}2m(1)\\ \bar{4}m2(1)\end{array}\right.;\ \dfrac{\mathbf{4}}{\boldsymbol{m}}\mathbf{mm}(m..)$ |
| 16 | Ditetragonal dipyramid | Edge-truncated tetragonal prism | 16 | $\dfrac{4}{m}mm$ | $\dfrac{\mathbf{4}}{\boldsymbol{m}}\mathbf{mm(1)}$ |
| 17 | Trigonal pyramid | Trigon | 3 | $3m$ | $3(1);\ \left\{\begin{array}{l}\mathbf{3m1}(.m.)\\ \mathbf{31m}(..m)\\ \mathbf{3m}\ (.m)\end{array}\right.$ |

**Table 3.2.1.3 (continued)**

| No. | Crystal form | Point form | Number of faces or points | Eigensymmetry | Generating point groups with oriented face (site) symmetries between parentheses |
|---|---|---|---|---|---|
| 18 | Trigonal prism | Trigon through origin | 3 | $\overline{6}2m$ | $3(1)$; $\begin{cases} \mathbf{321}(.2.) \\ \mathbf{312}(..2) \\ \mathbf{32}\ (.2) \end{cases}$ $\begin{cases} 3m1(.m.) \\ 31m(..m) \\ 3m\ (.m) \end{cases}$; $\overline{6}(\boldsymbol{m}..)$; $\begin{cases} \overline{\mathbf{6}}\boldsymbol{m2}(\boldsymbol{mm2}) \\ \overline{\mathbf{6}}\boldsymbol{2m}(\boldsymbol{m2m}) \end{cases}$ |
| 19 | Trigonal trapezohedron | Twisted trigonal antiprism | 6 | 32 | $\begin{cases} \mathbf{321(1)} \\ \mathbf{312(1)} \\ \mathbf{32}\ \mathbf{(1)} \end{cases}$ |
| 20 | Ditrigonal pyramid | Truncated trigon | 6 | $3m$ | $\begin{cases} \boldsymbol{3m1(1)} \\ \boldsymbol{31m(1)} \\ \boldsymbol{3m}\ \mathbf{(1)} \end{cases}$ |
| 21 | Rhombohedron | Trigonal antiprism | 6 | $\overline{3}m$ | $\overline{3}(\mathbf{1})$; $\begin{cases} 321(1) \\ 312(1) \\ 32\ (1) \end{cases}$ $\begin{cases} \overline{\mathbf{3}}\boldsymbol{m1}(.m.) \\ \overline{\mathbf{3}}\boldsymbol{1m}(..m) \\ \overline{\mathbf{3}}\boldsymbol{m}\ (.m) \end{cases}$ |
| 22 | Ditrigonal prism | Truncated trigon through origin | 6 | $\overline{6}2m$ | $\begin{cases} 321(1) \\ 312(1) \\ 32\ (1) \end{cases}$ $\begin{cases} 3m1(1) \\ 31m(1) \\ 3m\ (1) \end{cases}$; $\begin{cases} \overline{\mathbf{6}}\boldsymbol{m2}(\boldsymbol{m}..) \\ \overline{\mathbf{6}}\boldsymbol{2m}(\boldsymbol{m}..) \end{cases}$ |
| 23 | Hexagonal pyramid | Hexagon | 6 | $6mm$ | $\begin{cases} 3m1(1) \\ 31m(1) \\ 3m\ (1) \end{cases}$; $\mathbf{6(1)}$; $\boldsymbol{6mm}(..m,.m.)$ |
| 24 | Trigonal dipyramid | Trigonal prism | 6 | $\overline{6}2m$ | $\begin{cases} 321(1) \\ 312(1) \\ 32\ (1) \end{cases}$; $\overline{6}(\mathbf{1})$; $\begin{cases} \overline{\mathbf{6}}\boldsymbol{m2}(.m.) \\ \overline{\mathbf{6}}\boldsymbol{2m}(..m) \end{cases}$ |
| 25 | Hexagonal prism | Hexagon through origin | 6 | $\dfrac{6}{m}mm$ | $\overline{3}(1)$; $\begin{cases} 321(1) \\ 312(1) \\ 32\ (1) \end{cases}$ $\begin{cases} 3m1(1) \\ 31m(1) \\ 3m\ (1) \end{cases}$; $\ddagger\begin{cases} \overline{\mathbf{3}}\boldsymbol{m1}(.2.)\ \text{and}\ \overline{\mathbf{3}}\boldsymbol{m1}(.m.) \\ \overline{\mathbf{3}}\boldsymbol{1m}(..2)\ \text{and}\ \overline{\mathbf{3}}\boldsymbol{1m}(..m) \\ \overline{\mathbf{3}}\boldsymbol{m}(.2)\ \text{and}\ \overline{\mathbf{3}}\boldsymbol{m}(.m) \end{cases}$ $6(1)$; $\dfrac{6}{m}(\boldsymbol{m}..)$; $\mathbf{622}(.2.,..2)$; $6mm(..m,.m.)$; $\begin{cases} \overline{\mathbf{6}}\boldsymbol{m2}(\boldsymbol{m}..) \\ \overline{\mathbf{6}}\boldsymbol{2m}(\boldsymbol{m}..) \end{cases}$; $\dfrac{6}{m}\boldsymbol{mm}(\boldsymbol{m2m},\boldsymbol{mm2})$ |
| 26 | Ditrigonal scalenohedron or hexagonal scalenohedron | Trigonal antiprism sliced off by pinacoid | 12 | $\overline{3}m$ | $\begin{cases} \overline{\mathbf{3}}\boldsymbol{m1(1)} \\ \overline{\mathbf{3}}\boldsymbol{1m(1)} \\ \overline{\mathbf{3}}\boldsymbol{m}\ \mathbf{(1)} \end{cases}$ |
| 27 | Hexagonal trapezohedron | Twisted hexagonal antiprism | 12 | 622 | $\mathbf{622(1)}$ |
| 28 | Dihexagonal pyramid | Truncated hexagon | 12 | $6mm$ | $\boldsymbol{6mm(1)}$ |
| 29 | Ditrigonal dipyramid | Edge-truncated trigonal prism | 12 | $\overline{6}2m$ | $\begin{cases} \overline{\mathbf{6}}\boldsymbol{m2(1)} \\ \overline{\mathbf{6}}\boldsymbol{2m(1)} \end{cases}$ |
| 30 | Dihexagonal prism | Truncated hexagon | 12 | $\dfrac{6}{m}mm$ | $\begin{cases} \overline{3}m1(1) \\ \overline{3}1m(1) \\ \overline{3}m\ (1) \end{cases}$; $622(1)$; $6mm(1)$; $\dfrac{6}{m}\boldsymbol{mm}(\boldsymbol{m}..)$ |
| 31 | Hexagonal dipyramid | Hexagonal prism | 12 | $\dfrac{6}{m}mm$ | $\begin{cases} \overline{3}m1(1) \\ \overline{3}1m(1) \\ \overline{3}m\ (1) \end{cases}$; $\dfrac{6}{m}(1)$; $622(1)\dagger$; $\begin{cases} \overline{6}m2(1) \\ \overline{6}2m(1) \end{cases}$; $\dfrac{6}{m}\boldsymbol{mm}(..\boldsymbol{m},.\boldsymbol{m}.)$ |

**Table 3.2.1.3 (continued)**

| No. | Crystal form | Point form | Number of faces or points | Eigensymmetry | Generating point groups with oriented face (site) symmetries between parentheses |
|---|---|---|---|---|---|
| 32 | Dihexagonal dipyramid | Edge-truncated hexagonal prism | 24 | $\frac{6}{m}mm$ | $\frac{6}{m}mm(1)$ |
| 33 | Tetrahedron | Tetrahedron | 4 | $\bar{4}3m$ | $23(.3.)$; $\bar{4}3m(.3m)$ |
| 34 | Cube or hexahedron | Octahedron | 6 | $m\bar{3}m$ | $23(2..)$; $m\bar{3}(2mm..)$; $432(4..)$; $\bar{4}3m(2.mm)$; $m\bar{3}m(4m.m)$ |
| 35 | Octahedron | Cube | 8 | $m\bar{3}m$ | $m\bar{3}(.3.)$; $432(.3.)$; $m\bar{3}m(.3m)$ |
| 36 | Pentagon-tritetrahedron or tetartoid or tetrahedral pentagon-dodecahedron | Snub tetrahedron (= pentagon-tritetrahedron + two tetrahedra) | 12 | 23 | $23(1)$ |
| 37 | Pentagon-dodecahedron or dihexahedron or pyritohedron | Irregular icosahedron (= pentagon-dodecahedron + octahedron) | 12 | $m\bar{3}$ | $23(1)$; $m\bar{3}(m..)$ |
| 38 | Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron | Cube and two tetrahedra | 12 | $\bar{4}3m$ | $23(1)$; $\bar{4}3m(..m)$ |
| 39 | Trigon-tritetrahedron or tristetrahedron | Tetrahedron truncated by tetrahedron | 12 | $\bar{4}3m$ | $23(1)$; $\bar{4}3m(..m)$ |
| 40 | Rhomb-dodecahedron | Cuboctahedron | 12 | $m\bar{3}m$ | $23(1)$; $m\bar{3}(m..)$; $432(..2)$; $\bar{4}3m(..m)$; $m\bar{3}m(m.m2)$ |
| 41 | Didodecahedron or diploid or dyakisdodecahedron | Cube & octahedron & pentagon-dodecahedron | 24 | $m\bar{3}$ | $m\bar{3}(1)$ |
| 42 | Trigon-trioctahedron or trisoctahedron | Cube truncated by octahedron | 24 | $m\bar{3}m$ | $m\bar{3}(1)$; $432(1)$; $m\bar{3}m(..m)$ |
| 43 | Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron | Cube & octahedron & rhomb-dodecahedron | 24 | $m\bar{3}m$ | $m\bar{3}(1)$; $432(1)$; $m\bar{3}m(..m)$ |
| 44 | Pentagon-trioctahedron or gyroid | Cube + octahedron + pentagon-trioctahedron | 24 | 432 | $432(1)$ |
| 45 | Hexatetrahedron or hexakistetrahedron | Cube truncated by two tetrahedra | 24 | $\bar{4}3m$ | $\bar{4}3m(1)$ |
| 46 | Tetrahexahedron or tetrakishexahedron | Octahedron truncated by cube | 24 | $m\bar{3}m$ | $432(1)$; $\bar{4}3m(1)$; $m\bar{3}m(m..)$ |
| 47 | Hexaoctahedron or hexakisoctahedron | Cube truncated by octahedron and by rhomb-dodecahedron | 48 | $m\bar{3}m$ | $m\bar{3}m(1)$ |

† These limiting forms occur in three or two non-equivalent orientations (different types of limiting forms); *cf.* Table 3.2.3.2.   ‡ In point groups $\bar{4}2m$ and $\bar{3}m$, the tetragonal prism and the hexagonal prism occur twice, as a 'basic special form' and as a 'limiting special form'. In these cases, the point groups are listed twice, as '$\bar{4}2m(.2.)$ and $\bar{4}2m(..m)$' and as '$\bar{3}m1(.2.)$ and $\bar{3}m1(.m.)$'.

hedry $6/mmm$ has to be taken). Different types of limiting forms may have the same eigensymmetry and the same topology, as shown by the examples below. The occurrence of two topologically different polyhedra as two 'realizations' of one type of limiting form in point groups 23, $m\bar{3}$ and 432 is explained below in Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).

*Examples*
(1) In point group 32, the limiting general crystal forms are of four types:
  (i) ditrigonal prisms, eigensymmetry $\bar{6}2m$ (face poles on horizontal mirror plane of holohedry $6/mmm$);
  (ii) trigonal dipyramids, eigensymmetry $\bar{6}2m$ (face poles on one kind of vertical mirror plane);

(iii) rhombohedra, eigensymmetry $\bar{3}m$ (face poles on second kind of vertical mirror plane);
(iv) hexagonal prisms, eigensymmetry $6/mmm$ (face poles on horizontal twofold axes).

Types (i) and (ii) have the same eigensymmetry but different topologies; types (i) and (iv) have the same topology but different eigensymmetries; type (iii) differs from the other three types in both eigensymmetry and topology.

(2) In point group 222, the face poles of the three types of general limiting forms, rhombic prisms, are located on the three (non-equivalent) symmetry planes of the holohedry *mmm*. Geometrically, the axes of the prisms are directed along the three non-equivalent orthorhombic symmetry directions. The three types of limiting forms have the same
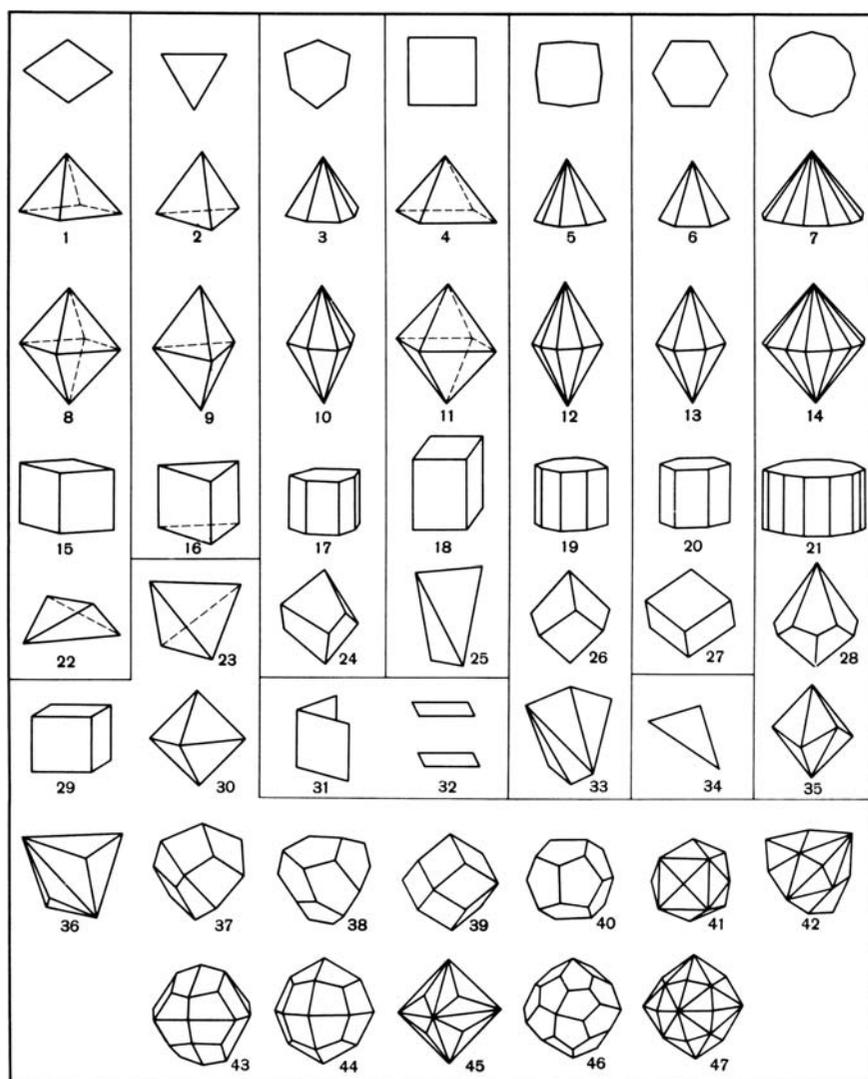
**Figure 3.2.1.1**
The 47 crystal forms that crystals may take (from Shubnikov & Koptsik, 1974, p. 74): (1)–(7) Pyramids: orthorhombic, trigonal, ditrigonal, tetragonal, ditetragonal, hexagonal, dihexagonal; (8)–(14) bipyramids of the same types; (15)–(21) prisms of the same types; (22), (23), (25) tetrahedra: orthorhombic, regular and tetragonal; (24), (26), (28) trapezohedra: trigonal, tetragonal, hexagonal: (27) rhombohedron; (34) scalene triangle; (33), (35) scalenohedra: tetragonal and ditrigonal; (31) dihedron (axial or non-axial); (32) pinacoid; (23), (29), (30), (36)–(47) simple forms of the cubic system: (23) tetrahedron; (29) hexahedron (cube); (30) octahedron; (36) trigonal tristetrahedron; (37) tetragonal tristetrahedron; (38) pentagonal tristetrahedron; (39) rhombic dodecahedron; (40) pentagonal dodecahedron; (41) tetrahexahedron; (42) hexatetrahedron; (43) didodecahedron; (44) tetragonal trisoctahedron; (45) trigonal trisoctahedron; (46) pentagonal trisoctahedron; (47) hexoctahedron. The central cross sections of all the figures above the stepped line dividing the table are the regular polygons indicated in the top row. Note that the numbers in this figure do not correspond to the numbers used in column 1 of Table 3.2.1.3.

eigensymmetry and the same topology but different orientations.

Similar cases occur in point groups 422 and 622 (*cf.* the first footnote to Table 3.2.1.3).

Not considered in this volume are limiting forms of another kind, namely those that require either special metrical conditions for the axial ratios or irrational indices or coordinates (which always can be closely approximated by rational values). For instance, a rhombic disphenoid can, for special axial ratios, appear as a tetragonal or even as a cubic tetrahedron; similarly, a rhombohedron can degenerate to a cube. For special irrational

indices, a ditetragonal prism changes to a (noncrystallographic) octagonal prism, a dihexagonal pyramid to a dodecagonal pyramid or a crystallographic pentagon-dodecahedron to a regular pentagon-dodecahedron. These kinds of limiting forms are listed by A. Niggli (1963).

In conclusion, each general or special Wyckoff position always contains one set of basic crystal (point) forms. In addition, it may contain one or more sets of limiting forms of different types. As a rule,[7] each type comprises polyhedra of the same eigensymmetry and topology and, hence, of the same name, for instance 'ditetragonal pyramid'. The name of the *basic general* forms is often used to designate the corresponding crystal class, for instance 'ditetragonal-pyramidal class'; some of these names are listed in Table 3.2.1.4.

### 3.2.1.2.3. Description of crystal and point forms

The main part of each point-group table in Section 3.2.3 describes the general and special *crystal and point forms* of that point group, in a manner analogous to the *positions* in a space group. The general Wyckoff position is given at the top, followed downwards by the special Wyckoff positions with decreasing multiplicity. Within each Wyckoff position, the first block of column 6 refers to the basic forms, the subsequent blocks list the various types of limiting form, if any.

The columns, from left to right, contain the following data (further details are to be found below in Section 3.2.1.2.4, *Notes on crystal and point forms*):

Column 1: *Multiplicity* of the 'Wyckoff position', *i.e.* the number of equivalent faces and points of a crystal or point form.

Column 2: *Wyckoff letter*. Each general or special 'Wyckoff position' is designated by a 'Wyckoff letter', analogous to the Wyckoff letter of a position in a space group (*cf.* Sections 1.4.4.2 and 2.1.3.11).

Column 3: *Face symmetry* or *site symmetry*, given in the form of an 'oriented point-group symbol', analogous to the oriented site-symmetry symbols of space groups (*cf.* Sections 1.4.4.2 and 2.1.3.12). The face symmetry is also the symmetry of etch pits, striations and other face markings. For the two-dimensional point groups, this column contains the *edge symmetry*, which can be either 1 or *m*.

Column 4: *Coordinates* $x, y, z$ of the symmetry-equivalent points of a point form.

Column 5: *Name of crystal form*. If more than one name is in common use, several are listed. The names of the limiting forms are also given. The crystal forms, their names, eigensymmetries and occurrence in the point groups are summarized in Table 3.2.1.3, which may be useful for determinative purposes, as explained in Sections 3.2.2.2 and 3.2.2.3. There are 47 different

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[7] For the exceptions in the cubic crystal system *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).

**Table 3.2.1.4**

Names and symbols of the 32 crystal classes

| System used in this volume | Point group | | Schoenflies symbol | Class names | |
|---|---|---|---|---|---|
| | International symbol | | | Groth (1921) | Friedel (1926) |
| | Short | Full | | | |
| Triclinic | 1 | 1 | $C_1$ | Pedial (asymmetric) | Hemihedry |
| | $\bar{1}$ | $\bar{1}$ | $C_i(S_2)$ | Pinacoidal | Holohedry |
| Monoclinic | 2 | 2 | $C_2$ | Sphenoidal | Holoaxial hemihedry |
| | $m$ | $m$ | $C_s(C_{1h})$ | Domatic | Antihemihedry |
| | $2/m$ | $\dfrac{2}{m}$ | $C_{2h}$ | Prismatic | Holohedry |
| Orthorhombic | 222 | 222 | $D_2(V)$ | Disphenoidal | Holoaxial hemihedry |
| | $mm2$ | $mm2$ | $C_{2v}$ | Pyramidal | Antihemihedry |
| | $mmm$ | $\dfrac{2\,2\,2}{m\,m\,m}$ | $D_{2h}(V_h)$ | Dipyramidal | Holohedry |
| Tetragonal | 4 | 4 | $C_4$ | Pyramidal | Tetartohedry with 4-axis |
| | $\bar{4}$ | $\bar{4}$ | $S_4$ | Disphenoidal | Sphenohedral tetartohedry |
| | $4/m$ | $\dfrac{4}{m}$ | $C_{4h}$ | Dipyramidal | Parahemihedry |
| | 422 | 422 | $D_4$ | Trapezohedral | Holoaxial hemihedry |
| | $4mm$ | $4mm$ | $C_{4v}$ | Ditetragonal-pyramidal | Antihemihedry with 4-axis |
| | $\bar{4}2m$ | $\bar{4}2m$ | $D_{2d}(V_d)$ | Scalenohedral | Sphenohedral antihemihedry |
| | $4/mmm$ | $\dfrac{4\,2\,2}{m\,m\,m}$ | $D_{4h}$ | Ditetragonal-dipyramidal | Holohedry |

| | | | | | *Hexagonal* | *Rhombohedral* |
|---|---|---|---|---|---|---|
| Trigonal | 3 | 3 | $C_3$ | Pyramidal | Ogdohedry | Tetartohedry |
| | $\bar{3}$ | $\bar{3}$ | $C_{3i}(S_6)$ | Rhombohedral | Paratetartohedry | Parahemihedry |
| | 32 | 32 | $D_3$ | Trapezohedral | Holoaxial tetartohedry with 3-axis | Holoaxial hemihedry |
| | $3m$ | $3m$ | $C_{3v}$ | Ditrigonal-pyramidal | Hemimorphic antitetartohedry | Antihemihedry |
| | $\bar{3}m$ | $\bar{3}\dfrac{2}{m}$ | $D_{3d}$ | Ditrigonal-scalenohedral | Parahemihedry with 3-axis | Holohedry |

| System used in this volume | Short | Full | Schoenflies symbol | Groth (1921) | Friedel (1926) |
|---|---|---|---|---|---|
| Hexagonal | 6 | 6 | $C_6$ | Pyramidal | Tetartohedry with 6-axis |
| | $\bar{6}$ | $\bar{6}$ | $C_{3h}$ | Trigonal-dipyramidal | Trigonohedral antitetartohedry |
| | $6/m$ | $\dfrac{6}{m}$ | $C_{6h}$ | Dipyramidal | Parahemihedry with 6-axis |
| | 622 | 622 | $D_6$ | Trapezohedral | Holoaxial hemihedry |
| | $6mm$ | $6mm$ | $C_{6v}$ | Dihexagonal-pyramidal | Antihemihedry with 6-axis |
| | $\bar{6}2m$ | $\bar{6}2m$ | $D_{3h}$ | Ditrigonal-dipyramidal | Trigonohedral antihemihedry |
| | $6/mmm$ | $\dfrac{6\,2\,2}{m\,m\,m}$ | $D_{6h}$ | Dihexagonal-dipyramidal | Holohedry |
| Cubic | 23 | 23 | $T$ | Tetrahedral-pentagondodecahedral (= tetartoidal) | Tetartohedry |
| | $m\bar{3}$ | $\dfrac{2}{m}\bar{3}$ | $T_h$ | Disdodecahedral (= diploidal) | Parahemihedry |
| | 432 | 432 | $O$ | Pentagon-icositetrahedral (= gyroidal) | Holoaxial hemihedry |
| | $\bar{4}3m$ | $\bar{4}3m$ | $T_d$ | Hexakistetrahedral (= hextetrahedral) | Antihemihedry |
| | $m\bar{3}m$ | $\dfrac{4}{m}\bar{3}\dfrac{2}{m}$ | $O_h$ | Hexakisoctahedral (= hexoctahedral) | Holohedry |

types of crystal form. Frequently, 48 are quoted because 'sphenoid' and 'dome' are considered as two different forms. It is customary, however, to regard them as the same form, with the name 'dihedron'.

*Name of point form* (printed in italics). There exists no general convention on the names of the point forms. Here, only one name is given, which does not always agree with that of other authors. The names of the point forms are also contained in Table 3.2.1.3.

Note that the same point form, 'line segment', corresponds to both sphenoid and dome.

Column 6: *Miller indices* (*hkl*) for the symmetry-equivalent faces (edges) of a crystal form. In the trigonal and hexagonal crystal systems, when referring to hexagonal axes, Bravais–Miller indices (*hkil*) are used, with $h + k + i = 0$.

With a few exceptions, the triplets of Miller indices (*hkl*) and point coordinates $x, y, z$ are arranged in such a way as to show

analogous sequences; they are both based on the same set of generators, as described in Sections 1.4.3 and 2.1.3.10. For all point groups, except those referred to a hexagonal coordinate system, the correspondence between the $(hkl)$ and the $x, y, z$ triplets is immediately obvious.[8]

The sets of symmetry-equivalent crystal faces also represent the sets of equivalent reciprocal-lattice points, as well as the sets of equivalent X-ray (neutron) reflections. This important aspect is treated in Klapper & Hahn (2010).

*Examples*

(1) In point group $\overline{4}$, the general crystal form $4b$ is listed as $(hkl)$ $(\overline{h}\overline{k}l)$ $(k\overline{h}\overline{l})$ $(\overline{k}h\overline{l})$: the corresponding general position $4h$ of the symmorphic space group $P\overline{4}$ reads $x, y, z$; $\overline{x}, \overline{y}, z$; $y, \overline{x}, \overline{z}$; $\overline{y}, x, \overline{z}$.

(2) In point group 3 (hexagonal axes), the general crystal form $3b$ is listed as $(hkil)$ $(ihkl)$ $(kihl)$ with $i = -(h + k)$; the corresponding general point form $3b$ is $x, y, z$; $\overline{y}, x - y, z$; $\overline{x} + y, \overline{x}, z$.

(3) The Miller indices of the *cubic point groups* are arranged in one, two or four blocks of $(3 \times 4)$ entries. The first block belongs to point group 23. The second block belongs to the diagonal twofold axes in 432 and $m\overline{3}m$ or to the diagonal mirror plane in $\overline{4}3m$. In point groups $m\overline{3}$ and $m\overline{3}m$, the lower one or two blocks are derived from the upper blocks by application of the inversion.

Further discussion of the data in Tables 3.2.3.1 and 3.2.3.2 as far as molecular symmetry is concerned can be found in Section 3.2.4.3.

### 3.2.1.2.4. Notes on crystal and point forms

(i) As mentioned in Section 3.2.1.1, each set of Miller indices of a given point group represents infinitely many face forms with the same name. Exceptions occur for the following cases.

Some special crystal forms occur with only *one* representative. Examples are the pinacoid {001}, the hexagonal prism {10$\overline{1}$0} and the cube {100}. The Miller indices of these forms consist of fixed numbers and signs and contain no variables.

In a few noncentrosymmetric point groups, a special crystal form is realized by *two* representatives: they are related by a centre of symmetry that is not part of the point-group symmetry. These cases are

(*a*) the two opposite, polar pedions (001) and (00$\overline{1}$);

(*b*) the two trigonal prisms {10$\overline{1}$0} and {$\overline{1}$010}; similarly for two dimensions;

(*c*) the two trigonal prisms {11$\overline{2}$0} and {$\overline{1}\overline{1}$20}; similarly for two dimensions;

(*d*) the positive and negative tetrahedra {111} and {$\overline{1}\overline{1}\overline{1}$}.

In the point-group tables, both representatives of these forms are listed, separated by 'or', for instance '(001) or (00$\overline{1}$)'.

(ii) In crystallography, the terms tetragonal, trigonal, hexagonal, as well as tetragon, trigon and hexagon, imply that the cross sections of the corresponding polyhedra, or the polygons, are *regular* tetragons (squares), trigons or hexagons. Similarly, ditetragonal, ditrigonal, dihexagonal, as well as ditetragon, ditrigon and dihexagon, refer to *semiregular* cross sections or polygons.

(iii) Crystal forms can be 'open' or 'closed'. A crystal form is 'closed' if its faces form a closed polyhedron; the minimum number of faces for a closed form is 4. Closed forms are disphenoids, dipyramids, rhombohedra, trapezohedra, scalenohedra and all cubic forms; open forms are pedions, pinacoids, sphenoids (domes), pyramids and prisms.

A point form is always closed. It should be noted, however, that a point form dual to a *closed* face form is a *three*-dimensional polyhedron, whereas the dual of an *open* face form is a *two*- or *one*-dimensional polygon, which, in general, is located 'off the origin' but may be centred at the origin (here called 'through the origin').

(iv) Crystal forms are well known; they are described and illustrated in many textbooks. Crystal forms are 'isohedral' polyhedra that have all faces equivalent but may have more than one kind of vertex; they include regular polyhedra. The in-sphere of the polyhedron touches all the faces.

Crystallographic point forms are less known; they are described in a few places only, notably by A. Niggli (1963), by Fischer *et al.* (1973), and by Burzlaff & Zimmermann (1977). The latter publication contains drawings of the polyhedra of all point forms. Point forms are 'isogonal' polyhedra (polygons) that have all vertices equivalent but may have more than one kind of face;[9] again, they include regular polyhedra. The circumsphere of the polyhedron passes through all the vertices.

In most cases, the names of the point-form polyhedra can easily be derived from the corresponding crystal forms: the duals of $n$-gonal pyramids are regular $n$-gons off the origin, those of $n$-gonal prisms are regular $n$-gons through the origin. The duals of di-$n$-gonal pyramids and prisms are truncated (regular) $n$-gons, whereas the duals of $n$-gonal dipyramids are $n$-gonal prisms.

In a few cases, however, the relations are not so evident. This applies mainly to some cubic point forms [see item (v) below]. A further example is the rhombohedron, whose dual is a trigonal antiprism (in general, the duals of $n$-gonal streptohedra are $n$-gonal antiprisms).[10] The duals of $n$-gonal trapezohedra are polyhedra intermediate between $n$-gonal prisms and $n$-gonal antiprisms; they are called here 'twisted $n$-gonal antiprisms' (example: point group 622). Finally, the duals of di-$n$-gonal scalenohedra are $n$-gonal antiprisms 'sliced off' perpendicular to the prism axis by the pinacoid {001}.[11]

(v) Some cubic point forms have to be described by 'combinations' of 'isohedral' polyhedra because no common

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[8] The matrices of corresponding triplets $(\tilde{h}\tilde{k}\tilde{l})$ and $\tilde{x}, \tilde{y}, \tilde{z}$, *i.e.* of triplets generated by the same symmetry operation from $(hkl)$ and $x, y, z$, are inverse to each other, provided the $x, y, z$ and $\tilde{x}, \tilde{y}, \tilde{z}$ are regarded as columns and the $(hkl)$ and $(\tilde{h}\tilde{k}\tilde{l})$ as rows: this is due to the contravariant and covariant nature of the point coordinates and Miller indices, respectively. Note that for orthogonal matrices the inverse matrix equals the transposed matrix; in crystallography, this applies to all coordinate systems (including the rhombohedral one), except for the hexagonal system. The matrices for the symmetry operations occurring in the crystallographic point groups are listed in Tables 1.2.2.1 and 1.2.2.2.

[9] Thus, the name 'prism' for a *point form* implies combination of the prism with a pinacoid.

[10] A tetragonal tetrahedron is a digonal streptohedron; hence, its dual is a 'digonal antiprism', which is again a tetragonal tetrahedron.

[11] The dual of a tetragonal (= di-digonal) scalenohedron is a 'digonal antiprism', which is 'cut off' by the pinacoid {001}.

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 dipyramid' $\{hhl\}$ for $\chi = 0°$ and 'rhombohedron' $\{h0l\}$ for $\chi = 60°$.

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

*Examples*

(1) A tetragonal dipyramid 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 $\overline{4}2m$.

(2) A tetragonal prism appears in point group $\overline{4}2m$ both as a basic special form (4*b*) and as a limiting special form (4*c*).

(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 $m\overline{3}m$ and $\overline{4}3m$, the two kinds of polyhedra represent two realizations of one *special* 'Wyckoff position'; hence, they have the same Wyckoff letter. In the groups 23, $m\overline{3}$ 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
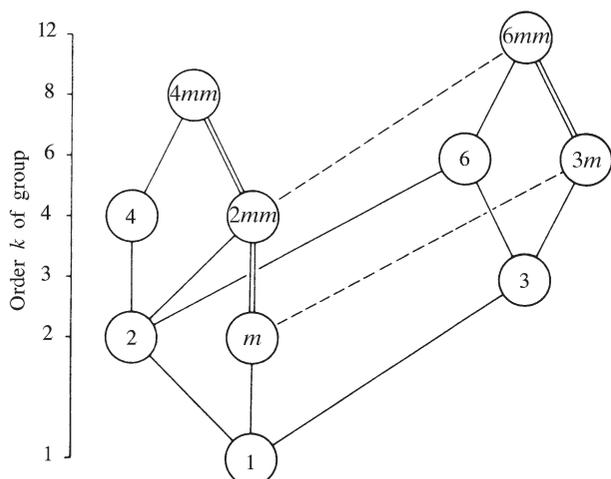
**Figure 3.2.1.2**
Maximal subgroups and minimal supergroups of the two-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. 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'.[12] 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 $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ of a group $\mathcal{P}$ are *conjugate* subgroups if $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ 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 $\mathcal{H}_j$: $W^{-1}\mathcal{H}_i W = \mathcal{H}_j$; *cf.* Sections 1.1.5 and 1.1.8.

*Examples*
(1) Point group 3*m* 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 3*m*. This set of conjugate subgroups is represented by *one* dashed line in Figs. 3.2.1.2 and 3.2.1.3.

[12] 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° 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.
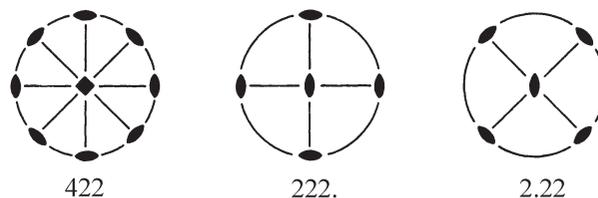


(2) Similarly, group 432 has one maximal normal subgroup, 23.

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.
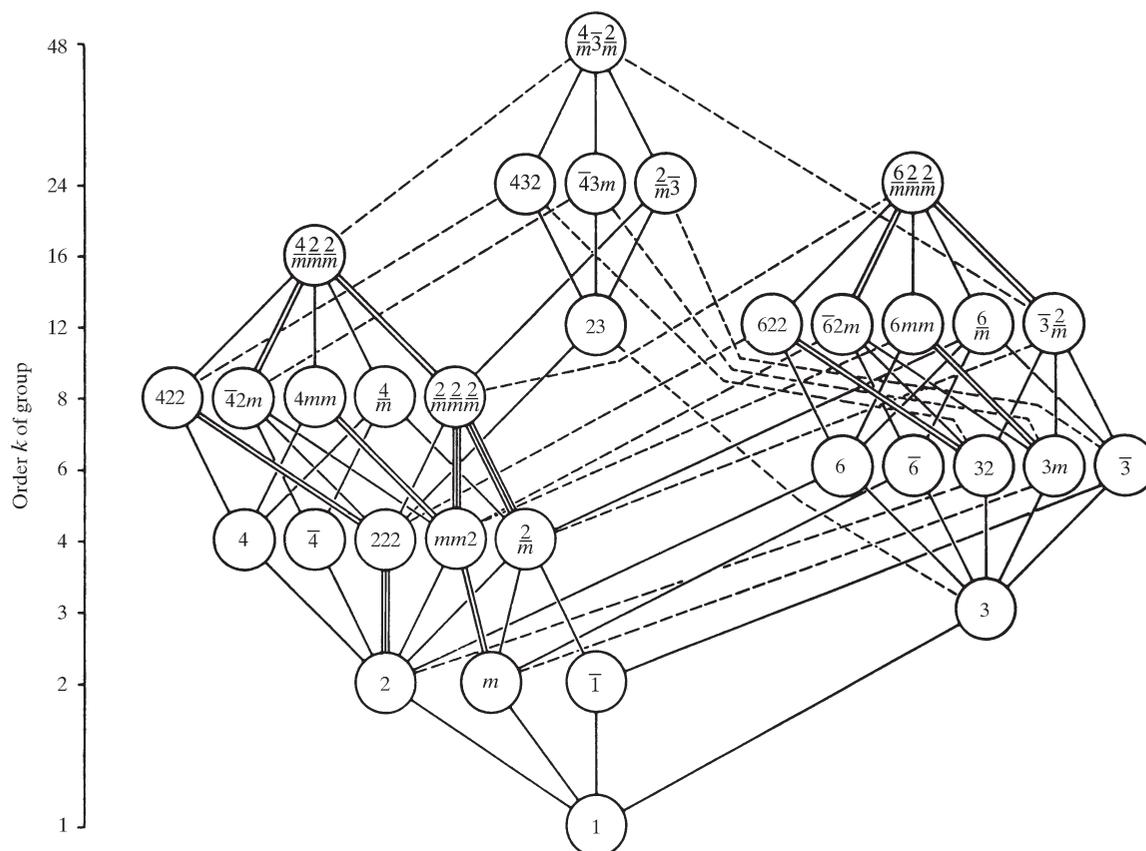
**Figure 3.2.1.3**
Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left. Full Hermann–Mauguin symbols are used.

Because of the infinite number of these groups only *classes of general point groups* (*general classes*)[13] can be listed. They are grouped into *general systems*, which are similar to the crystal systems. The 'general classes' are of two kinds: in the cubic, icosahedral, circular, cylindrical and spherical system, each general class contains *one* point group only, whereas in the 4$N$-gonal, $(2N + 1)$-gonal and $(4N + 2)$-gonal system, each general class contains *infinitely* many point groups, which differ in their principal $n$-fold symmetry axis, with $n = 4, 8, 12, \ldots$ for the 4$N$-gonal system, $n = 1, 3, 5, \ldots$ for the $(2N + 1)$-gonal system and $n = 2, 6, 10, \ldots$ for the $(4N + 2)$-gonal system.

Furthermore, some general point groups are of order infinity because they contain symmetry axes (rotation or rotoinversion axes) of order infinity[14] ($\infty$-fold axes). These point groups occur in the circular system (two dimensions) and in the cylindrical and spherical systems (three dimensions).

The Hermann–Mauguin and Schoenflies symbols for the general point groups follow the rules of the crystallographic point groups (*cf.* Sections 1.4.1, 2.1.3.4 and 3.3.1). This extends also to the infinite groups where symbols like $\infty m$ or $C_{\infty v}$ are immediately obvious.

In *two dimensions* (Table 3.2.1.5), the eight general classes are collected into three systems. Two of these, the 4$N$-gonal and the $(4N + 2)$-gonal systems, contain only point groups of finite order with one $n$-fold rotation point each. These systems are generalizations of the square and hexagonal crystal systems. The circular system consists of two infinite point groups, with one $\infty$-fold rotation point each.

In *three dimensions* (Table 3.2.1.6), the 33 general classes are collected into seven systems. Three of these, the 4$N$-gonal, the $(2N + 1)$-gonal and the $(4N + 2)$-gonal systems,[15] contain only point groups of finite order with one principal $n$-fold symmetry axis each. These systems are generalizations of the tetragonal, trigonal and hexagonal crystal systems (*cf.* Table 3.2.3.2). The five cubic groups are well known as crystallographic groups. The two icosahedral groups of orders 60 and 120, characterized by special combinations of twofold, threefold and fivefold symmetry axes, are discussed in more detail below. The groups of the cylindrical and the spherical systems are all of order infinity; they describe the symmetries of cylinders, cones, rotation ellipsoids, spheres *etc.*[16]

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[13] The 'classes of general point groups' are not the same as the commonly used 'crystal classes' because some of them contain point groups of *different orders*. All these orders, however, follow a common scheme. In this sense, the 'general classes' are an extension of the concept of (geometric) crystal classes. For example, the general class *nmm* of the 4$N$-gonal system contains the point groups 4$mm$ (tetragonal), 8$mm$ (octagonal), 12$mm$ (dodecagonal), 16$mm$ *etc.*

[14] The axes of order infinity, as considered here, do not correspond to cyclic groups (as do the axes of finite order) because there is no smallest rotation from which all other rotations can be derived as higher powers, *i.e.* by successive application. Instead, rotations of all possible angles exist. Nevertheless, it is customary to symbolize these axes as $\infty$ or $C_\infty$; note that the Hermann–Mauguin symbols $\infty/m$ and $\overline{\infty}$ are equivalent, and so are the Schoenflies symbols $C_{\infty h}$, $S_\infty$ and $C_{\infty i}$. (There exist also axes of order infinity that do correspond to cyclic groups, namely axes based upon smallest rotations with irrational values of the rotation angle.)

[15] Here, the $(2N + 1)$-gonal and the $(4N + 2)$-gonal systems are distinguished in order to bring out the analogy with the trigonal and the hexagonal crystal systems. They could equally well be combined into one, in correspondence with the hexagonal 'crystal family' (*cf.* Sections 1.3.4.4 and 2.1.1).

[16] The terms 'rotating' and 'stationary' in the circular, cylindrical and spherical systems do not imply any relation to dynamical properties (motions) of crystals or molecules. They only serve to illustrate the absence (group $\infty$) or presence ($\infty m$, $\overline{\infty}m$) of 'vertical' mirror planes in these groups or order $\infty$.

**Table 3.2.1.5**
Classes of general point groups in two dimensions ($N$ = integer $\geq 0$)

| General Hermann–Mauguin symbol | Order of group | General edge form | General point form | Crystallographic groups |
|---|---|---|---|---|
| $4N$-gonal system ($n$-fold rotation point with $n = 4N$) | | | | |
| $n$ | $n$ | Regular $n$-gon | Regular $n$-gon | 4 |
| $nmm$ | $2n$ | Semiregular di-$n$-gon | Truncated $n$-gon | $4mm$ |
| $(4N + 2)$-gonal system ($n$-fold or $\frac{1}{2}n$-fold rotation point with $n = 4N + 2$) | | | | |
| $\frac{1}{2}n$ | $\frac{1}{2}n$ | Regular $\frac{1}{2}n$-gon | Regular $\frac{1}{2}n$-gon | 1, 3 |
| $\frac{1}{2}nm$ | $n$ | Semiregular di-$\frac{1}{2}n$-gon | Truncated $\frac{1}{2}n$-gon | $m$, $3m$ |
| $n$ | $n$ | Regular $n$-gon | Regular $n$-gon | 2, 6 |
| $nmm$ | $2n$ | Semiregular di-$n$-gon | Truncated $n$-gon | $2mm$, $6mm$ |
| Circular system† | | | | |
| $\infty$ | $\infty$ | Rotating circle | Rotating circle | – |
| $\infty m$ | $\infty$ | Stationary circle | Stationary circle | – |

† A rotating circle has no mirror lines; there exist two enantiomorphic circles with opposite senses of rotation. A stationary circle has infinitely many mirror lines through its centre.

It is possible to define the three-dimensional point groups on the basis of either rotoinversion axes $\bar{n}$ or rotoreflection axes $\tilde{n}$. The equivalence between these two descriptions is apparent from the following examples:

$$n = 4N: \quad \bar{4} = \tilde{4} \quad\quad \bar{8} = \tilde{8} \quad\quad \ldots \quad \bar{n} = \tilde{n}$$
$$n = 2N + 1: \quad \bar{1} = \tilde{2} \quad\quad \bar{3} = \tilde{6} = 3 \times \bar{1} \quad \ldots \quad \bar{n} = \widetilde{2n} = n \times \bar{1}$$
$$n = 4N + 2: \quad \bar{2} = \tilde{1} = m \quad \bar{6} = \tilde{3} = 3/m \quad \ldots \quad \bar{n} = \tilde{\frac{1}{2}}n = \frac{1}{2}n/m.$$

In the present tables, the standard convention of using roto-inversion axes is followed.

Tables 3.2.1.5 and 3.2.1.6 contain for each class its general Hermann–Mauguin and Schoenflies symbols, the group order and the names of the general face form and its dual, the general point form.[17] Special and limiting forms are not given, nor are 'Miller indices' ($hkl$) and point coordinates $x, y, z$. They can be derived easily from Tables 3.2.3.1 and 3.2.3.2 for the crystallographic groups.[18]

### 3.2.1.4.2. The two icosahedral groups

The two point groups 235 and $m\bar{3}\bar{5}$ of the icosahedral system (orders 60 and 120) are of particular interest among the noncrystallographic groups because of the occurrence of fivefold axes and their increasing importance as symmetries of molecules (viruses), of quasicrystals, and as approximate local site symmetries in crystals (alloys, $B_{12}$ icosahedron). Furthermore, they contain as special forms the two noncrystallographic *platonic solids*, the regular icosahedron (20 faces, 12 vertices) and its dual, the regular pentagon-dodecahedron (12 faces, 20 vertices).

The icosahedral groups (*cf.* diagrams in Table 3.2.3.3) are characterized by six fivefold axes that include angles of 63.43°. Each fivefold axis is surrounded by five threefold and five twofold axes, with angular distances of 37.38° between a fivefold and a threefold axis and of 31.72° between a fivefold and a twofold axis. The angles between neighbouring threefold axes are 41.81°,

between neighbouring twofold axes 36°. The smallest angle between a threefold and a twofold axis is 20.90°.

Each of the six fivefold axes is perpendicular to five twofold axes; there are thus six maximal conjugate pentagonal subgroups of types 52 (for 235) and $\bar{5}m$ (for $m\bar{3}\bar{5}$) with index [6]. Each of the ten threefold axes is perpendicular to three twofold axes, leading to ten maximal conjugate trigonal subgroups of types 32 (for 235) and $\bar{3}m$ (for $m\bar{3}\bar{5}$) with index [10]. There occur, furthermore, five maximal conjugate cubic subgroups of types 23 (for 235) and $m\bar{3}$ (for $m\bar{3}\bar{5}$) with index [5].

The two icosahedral groups are listed in Table 3.2.3.3, in a form similar to the cubic point groups in Table 3.2.3.2. Each group is illustrated by stereographic projections of the symmetry elements and the general face poles (general points); the complete sets of symmetry elements are listed below the stereograms. Both groups are referred to a cubic coordinate system, with the coordinate axes along three twofold rotation axes and with four threefold axes along the body diagonals. This relation is well brought out by symbolizing these groups as 235 and $m\bar{3}\bar{5}$ instead of the customary symbols 532 and $\bar{5}\bar{3}m$.

The table contains also the multiplicities, the Wyckoff letters and the names of the general and special face forms and their duals, the point forms, as well as the oriented face- and site-symmetry symbols. In the icosahedral 'holohedry' $m\bar{3}\bar{5}$, the *special* 'Wyckoff position' 60$d$ occurs in three realizations, *i.e.* with three types of polyhedra. In 235, however, these three types of polyhedra are different realizations of the limiting *general* forms, which depend on the location of the poles with respect to the axes 2, 3 and 5. For this reason, the three entries are connected by braces; *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).

Not included are the sets of equivalent Miller indices and point coordinates. Instead, only the 'initial' triplets ($hkl$) and $x, y, z$ for each type of form are listed. The complete sets of indices and coordinates can be obtained in two steps[19] as follows:

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[17] The noncrystallographic face and point forms are extensions of the corresponding crystallographic forms: *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*. The name *streptohedron* applies to the general face forms of point groups $\bar{n}$ with $n = 4N$ and $n = 2N + 1$; it is thus a generalization of the tetragonal disphenoid or tetragonal tetrahedron ($\bar{4}$) and the rhombohedron ($\bar{3}$).
[18] The term 'Miller indices' is used here also for the noncrystallographic point groups. Note that these indices do not have to be integers or rational numbers, as for the crystallographic point groups. Irrational indices, however, can always be closely approximated by integers, quite often even by small integers.

[19] A one-step procedure applies to the icosahedral 'Wyckoff position' 12$a$, the face poles and points of which are located on the fivefold axes. Here, step (ii) is redundant and can be omitted. The forms $\{01\tau\}$ and $0, y, \tau y$ are contained in the cubic point groups 23 and $m\bar{3}$ and in the cubic space groups $P23$ and $Pm\bar{3}$ as limiting cases of Wyckoff positions$\{0kl\}$ and $0, y, z$ with specialized (irrational) values of the indices and coordinates. In geometric terms, the regular pentagon-dodecahedron is a noncrystallographic 'limiting polyhedron' of the 'crystallographic' pentagon-dodecahedron and the regular icosahedron is a 'limiting polyhedron' of the 'irregular' icosahedron (*cf.* Section 3.2.1.2.2, *Crystal and point forms*).

**Table 3.2.1.6**

Classes of general point groups in three dimensions ($N$ = integer $\geq 0$)

| Short general Hermann–Mauguin symbol, followed by full symbol where different | Schoenflies symbol | Order of group | General face form | General point form | Crystallographic groups |
|---|---|---|---|---|---|
| **4N-gonal system (single n-fold symmetry axis with $n = 4N$)** | | | | | |
| $n$ | $C_n$ | $n$ | $n$-gonal pyramid | Regular $n$-gon | 4 |
| $\bar{n}$ | $S_n$ | $n$ | $\frac{1}{2}n$-gonal streptohedron | $\frac{1}{2}n$-gonal antiprism | $\bar{4}$ |
| $n/m$ | $C_{nh}$ | $2n$ | $n$-gonal dipyramid | $n$-gonal prism | $4/m$ |
| $n22$ | $D_n$ | $2n$ | $n$-gonal trapezohedron | Twisted $n$-gonal antiprism | 422 |
| $nmm$ | $C_{nv}$ | $2n$ | Di-$n$-gonal pyramid | Truncated $n$-gon | $4mm$ |
| $\bar{n}2m$ | $D_{\frac{1}{2}nd}$ | $2n$ | $n$-gonal scalenohedron | $\frac{1}{2}n$-gonal antiprism sliced off by pinacoid | $\bar{4}2m$ |
| $n/mmm$, $\dfrac{n\,2\,2}{m\,m\,m}$ | $D_{nh}$ | $4n$ | Di-$n$-gonal dipyramid | Edge-truncated $n$-gonal prism | $4/mmm$ |
| **(2N + 1)-gonal system (single n-fold symmetry axis with $n = 2N + 1$)** | | | | | |
| $n$ | $C_n$ | $n$ | $n$-gonal pyramid | Regular $n$-gon | 1, 3 |
| $\bar{n} = n \times \bar{1}$ | $C_{ni}$ | $2n$ | $n$-gonal streptohedron | $n$-gonal antiprism | $\bar{1}$, $\bar{3} = 3 \times \bar{1}$ |
| $n2$ | $D_n$ | $2n$ | $n$-gonal trapezohedron | Twisted $n$-gonal antiprism | 32 |
| $nm$ | $C_{nv}$ | $2n$ | Di-$n$-gonal pyramid | Truncated $n$-gon | $3m$ |
| $\bar{n}m$, $\bar{n}\dfrac{2}{m}$ | $D_{nd}$ | $4n$ | Di-$n$-gonal scalenohedron | $n$-gonal antiprism sliced off by pinacoid | $\bar{3}m$ |
| **(4N + 2)-gonal system (single n-fold symmetry axis with $n = 4N + 2$)** | | | | | |
| $n$ | $C_n$ | $n$ | $n$-gonal pyramid | Regular $n$-gon | 2, 6 |
| $\bar{n} = \frac{1}{2}n/m$ | $C_{\frac{1}{2}nh}$ | $n$ | $\frac{1}{2}n$-gonal dipyramid | $\frac{1}{2}n$-gonal prism | $\bar{2} \equiv m$, $\bar{6} \equiv 3/m$ |
| $n/m$ | $C_{nh}$ | $2n$ | $n$-gonal dipyramid | $n$-gonal prism | $2/m$, $6/m$ |
| $n22$ | $D_n$ | $2n$ | $n$-gonal trapezohedron | Twisted $n$-gonal antiprism | 222, 622 |
| $nmm$ | $C_{nv}$ | $2n$ | Di-$n$-gonal pyramid | Truncated $n$-gon | $mm2$, $6mm$ |
| $\bar{n}2m = \frac{1}{2}n/m2m$ | $D_{\frac{1}{2}nh}$ | $2n$ | Di-$\frac{1}{2}n$-gonal dipyramid | Truncated $\frac{1}{2}n$-gonal prism | $\bar{6}2m$ |
| $n/mmm$, $\dfrac{n\,2\,2}{m\,m\,m}$ | $D_{nh}$ | $4n$ | Di-$n$-gonal dipyramid | Edge-truncated $n$-gonal prism | $mmm$, $6/mmm$ |
| **Cubic system (for details see Table 3.2.3.2)** | | | | | |
| 23 | $T$ | 12 | Pentagon-tritetrahedron | Snub tetrahedron | 23 |
| $m\bar{3}$, $\dfrac{2}{m}\bar{3}$ | $T_h$ | 24 | Didodecahedron | Cube & octahedron & pentagon-dodecahedron | $m\bar{3}$ |
| 432 | $O$ | 24 | Pentagon-trioctahedron | Snub cube | 432 |
| $\bar{4}3m$ | $T_d$ | 24 | Hexatetrahedron | Cube truncated by two tetrahedra | $\bar{4}3m$ |
| $m\bar{3}m$, $\dfrac{4}{m}\bar{3}\dfrac{2}{m}$ | $O_h$ | 48 | Hexaoctahedron | Cube truncated by octahedron and by rhomb-dodecahedron | $m\bar{3}m$ |
| **Icosahedral system† (for details see Table 3.2.3.3)** | | | | | |
| 235 | $I$ | 60 | Pentagon-hexecontahedron | Snub pentagon-dodecahedron | – |
| $m\bar{3}\bar{5}$, $\dfrac{2}{m}\bar{3}\bar{5}$ | $I_h$ | 120 | Hecatonicosahedron | Pentagon-dodecahedron truncated by icosahedron and by rhomb-triacontahedron | – |
| **Cylindrical system‡** | | | | | |
| $\infty$ | $C_\infty$ | $\infty$ | Rotating cone | Rotating circle | – |
| $\infty/m \equiv \overline{\infty}$ | $C_{\infty h} \equiv S_\infty \equiv C_{\infty i}$ | $\infty$ | Rotating double cone | Rotating finite cylinder | – |
| $\infty 2$ | $D_\infty$ | $\infty$ | 'Anti-rotating' double cone | 'Anti-rotating' finite cylinder | – |
| $\infty m$ | $C_{\infty v}$ | $\infty$ | Stationary cone | Stationary circle | – |
| $\infty/mm \equiv \overline{\infty}m$, $\dfrac{\infty}{m}\dfrac{2}{m} \equiv \overline{\infty}\dfrac{2}{m}$ | $D_{\infty h} = D_{\infty d}$ | $\infty$ | Stationary double cone | Stationary finite cylinder | – |
| **Spherical system§** | | | | | |
| $2\infty$, $\infty\infty\infty$ | $K$ | $\infty$ | Rotating sphere | Rotating sphere | – |
| $m\overline{\infty}$, $\dfrac{2}{m}\overline{\infty}$, $\infty\infty\infty m$ | $K_h$ | $\infty$ | Stationary sphere | Stationary sphere | – |

† The Hermann–Mauguin symbols of the two icosahedral point groups are often written as 532 and $\bar{5}\bar{3}m$ (see text).   ‡ Rotating and 'anti-rotating' forms in the cylindrical system have no 'vertical' mirror planes, whereas stationary forms have infinitely many vertical mirror planes. In classes $\infty$ and $\infty 2$, enantiomorphism occurs, *i.e.* forms with opposite senses of rotation. Class $\infty/m \equiv \overline{\infty}$ exhibits no enantiomorphism due to the centre of symmetry, even though the double cone is rotating in one direction. This can be understood as follows: The handedness of a rotating cone depends on the sense of rotation with respect to the axial direction from the base to the tip of the cone. Thus, the rotating double cone consists of two cones with opposite handedness and opposite orientations related by the (single) horizontal mirror plane. In contrast, the 'anti-rotating' double cone in class $\infty 2$ consists of two cones of equal handedness and opposite orientations, which are related by the (infinitely many) twofold axes. The term 'anti-rotating' means that upper and lower halves of the forms rotate in opposite directions.   § The spheres in class $2\infty$ of the spherical system must rotate around an axis with at least two different orientations, in order to suppress all mirror planes. This class exhibits enantiomorphism, *i.e.* it contains spheres with either right-handed or left-handed senses of rotation around the axes (*cf.* Section 3.2.2.4, *Optical properties*). The stationary spheres in class $m\overline{\infty}$ contain infinitely many mirror planes through the centres of the spheres. Group $2\infty$ is sometimes symbolized by $\infty\infty$; group $m\overline{\infty}$ by $\overline{\infty}\,\overline{\infty}$ or $\infty\infty m$. The symbols used here indicate the minimal symmetry necessary to generate the groups; they show, furthermore, the relation to the cubic groups. The Schoenflies symbol $K$ is derived from the German name *Kugelgruppe*.

(i) For the face forms the cubic point groups 23 and $m\overline{3}$ (Table 3.2.3.2), and for the point forms the cubic space groups $P23$ (195) and $Pm\overline{3}$ (200) have to be considered. For each 'initial' triplet $(hkl)$, the set of Miller indices of the (general or special) crystal form with the same face symmetry in 23 (for group 235) or $m\overline{3}$ (for $m\overline{3}\overline{5}$) is taken. For each 'initial' triplet $x, y, z$, the coordinate triplets of the (general or special) position with the same site symmetry in $P23$ or $Pm\overline{3}$ are taken.

(ii) To obtain the complete set of icosahedral Miller indices and point coordinates, the 'cubic' $(hkl)$ triplets (as rows) and $x, y, z$ triplets (as columns) have to be multiplied with the identity matrix and with

   (a) the matrices $\boldsymbol{Y}, \boldsymbol{Y}^2, \boldsymbol{Y}^3$ and $\boldsymbol{Y}^4$ for the Miller indices;

   (b) the matrices $\boldsymbol{Y}^{-1}, \boldsymbol{Y}^{-2}, \boldsymbol{Y}^{-3}$ and $\boldsymbol{Y}^{-4}$ for the point coordinates.

This sequence of matrices ensures the same correspondence between the Miller indices and the point coordinates as for the crystallographic point groups in Table 3.2.3.2.

The matrices[20] are

$$\boldsymbol{Y} = \boldsymbol{Y}^{-4} = \begin{pmatrix} \frac{1}{2} & g & G \\ g & G & -\frac{1}{2} \\ -G & \frac{1}{2} & g \end{pmatrix}, \quad \boldsymbol{Y}^2 = \boldsymbol{Y}^{-3} = \begin{pmatrix} -g & G & \frac{1}{2} \\ G & \frac{1}{2} & -g \\ -\frac{1}{2} & g & -G \end{pmatrix},$$

$$\boldsymbol{Y}^3 = \boldsymbol{Y}^{-2} = \begin{pmatrix} -g & G & -\frac{1}{2} \\ G & \frac{1}{2} & g \\ \frac{1}{2} & -g & -G \end{pmatrix}, \quad \boldsymbol{Y}^4 = \boldsymbol{Y}^{-1} = \begin{pmatrix} \frac{1}{2} & g & -G \\ g & G & \frac{1}{2} \\ G & -\frac{1}{2} & g \end{pmatrix},$$

with[21]

$$G = \frac{\sqrt{5}+1}{4} = \frac{\tau}{2} = \cos 36° = 0.80902 \simeq \frac{72}{89}$$

$$g = \frac{\sqrt{5}-1}{4} = \frac{\tau - 1}{2} = \cos 72° = 0.30902 \simeq \frac{17}{55}.$$

These matrices correspond to counter-clockwise rotations of 72, 144, 216 and 288° around a fivefold axis parallel to $[1\,\tau\,0]$.

The resulting indices $h, k, l$ and coordinates $x, y, z$ are irrational but can be approximated closely by rational (or integral) numbers. This explains the occurrence of almost regular icosahedra or pentagon-dodecahedra as crystal forms (for instance pyrite) or atomic groups (for instance $B_{12}$ icosahedron).

Further descriptions (including diagrams) of noncrystallographic groups are contained in papers by Nowacki (1933) and A. Niggli (1963) and in the textbooks by P. Niggli (1941, pp. 78–80, 96), Shubnikov & Koptsik (1974) and Vainshtein (1994). For the geometry of polyhedra, the well known books by H. S. M. Coxeter (especially Coxeter, 1973) are recommended.

### 3.2.1.4.3. Sub- and supergroups of the general point groups

In Figs. 3.2.1.4 to 3.2.1.6, the subgroup and supergroup relations between the two-dimensional and three-dimensional general point groups are illustrated. It should be remembered that the index of a group–subgroup relation between two groups of order infinity may be finite or infinite. For the two spherical
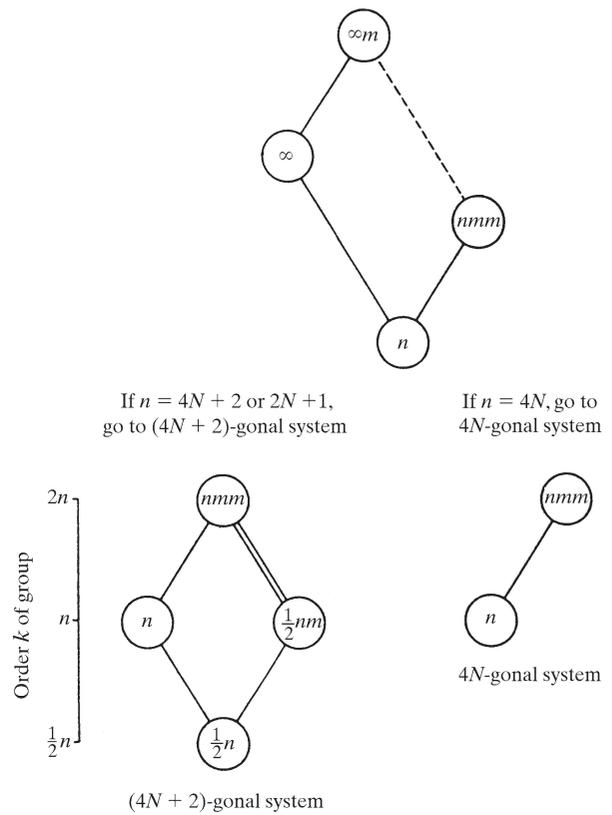


**Figure 3.2.1.4**
Subgroups and supergroups of the two-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, the orders are given on the left. Note that the subgroups of the two circular groups are not maximal and the diagram applies only to a specified value of $N$ (see text). For complete examples see Fig. 3.2.1.5.
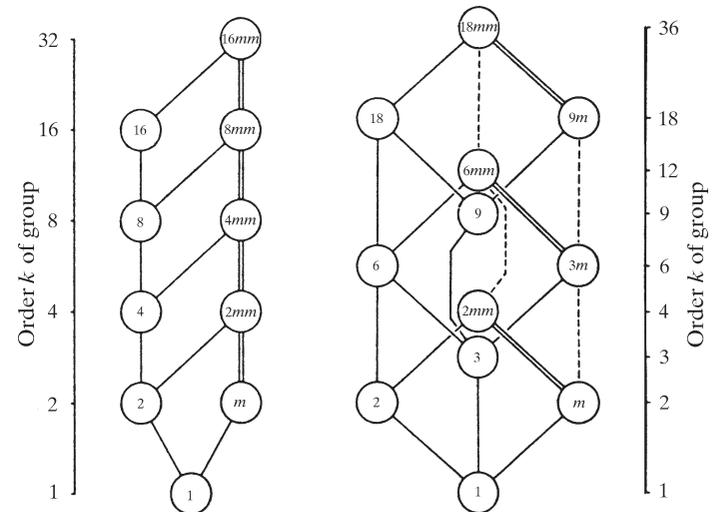


**Figure 3.2.1.5**
The subgroups of the two-dimensional general point groups $16mm$ ($4N$-gonal system) and $18mm$ [$(4N+2)$-gonal system, including the $(2N+1)$-gonal groups]. Compare with Fig. 3.2.1.4 which applies only to one value of $N$.

groups, for instance, the index is [2]; the cylindrical groups, on the other hand, are subgroups of index [∞] of the spherical groups.

Fig. 3.2.1.4 for *two dimensions* shows that the two circular groups ∞$m$ and ∞ have subgroups of types $nmm$ and $n$,
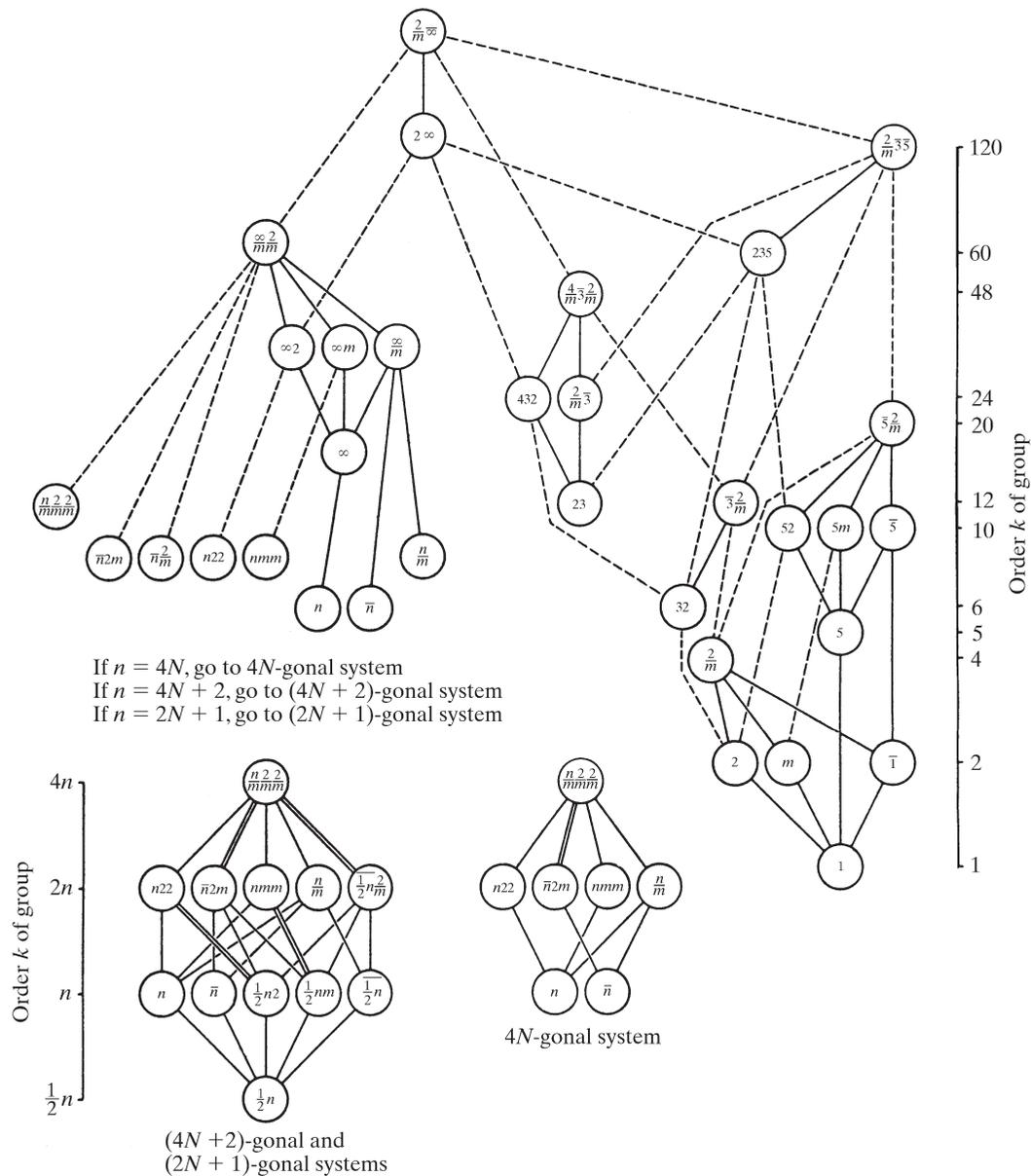
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**Figure 3.2.1.6**
Subgroups and supergroups of the three-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, the orders are given on the left and on the right. Note that the subgroups of the five cylindrical groups are not maximal and that the diagram applies only to a specified value of $N$ (see text). Only those crystallographic point groups are included that are maximal subgroups of noncrystallographic point groups, *cf.* Fig. 3.2.1.3. Full Hermann–Mauguin symbols are used.

respectively, each of index $[\infty]$. The order of the rotation point may be $n = 4N$, $n = 4N + 2$ or $n = 2N + 1$. In the first case, the subgroups belong to the $4N$-gonal system, in the latter two cases, they belong to the $(4N + 2)$-gonal system. [In the diagram of the $(4N + 2)$-gonal system, the $(2N + 1)$-gonal groups appear with the symbols $\frac{1}{2}nm$ and $\frac{1}{2}n$.] The subgroups of the circular groups are not maximal because for any given value of $N$ there exists a group with $N' = 2N$ which is both a subgroup of the circular group and a supergroup of the initial group.

The subgroup relations, for a specified value of $N$, within the $4N$-gonal and the $(4N + 2)$-gonal system, are shown in the lower part of the figure. They correspond to those of the crystallographic groups. A finite number of further maximal subgroups is obtained for lower values of $N$, until the crystallographic groups (Fig. 3.2.1.2) are reached. This is illustrated for both systems in Fig. 3.2.1.5.

Fig. 3.2.1.6 for *three dimensions* illustrates that the two spherical groups $2/m\overline{\infty}$ and $2\infty$ each have one infinite set of

cylindrical maximal conjugate subgroups, as well as one infinite set of cubic and one infinite set of icosahedral maximal finite conjugate subgroups, all of index $[\infty]$.

Each of the two icosahedral groups $235$ and $2/m\,\overline{3}\,\overline{5}$ has one set of five cubic, one set of six pentagonal and one set of ten trigonal maximal conjugate subgroups of indices $[5]$, $[6]$ and $[10]$, respectively (*cf.* Section 3.2.1.4.2, *The two icosahedral groups*); they are listed on the right of Fig. 3.2.1.6. For the crystallographic groups, Fig. 3.2.1.3 applies. The subgroup types of the five cylindrical point groups are shown in the upper left part of Fig. 3.2.1.6. As explained above for two dimensions, these subgroups are *not maximal* and of index $[\infty]$. Depending upon whether the main symmetry axis has the multiplicity $4N$, $4N + 2$ or $2N + 1$, the subgroups belong to the $4N$-gonal, $(4N + 2)$-gonal or $(2N + 1)$-gonal system.

The subgroup and supergroup relations within these three systems are displayed in the lower left part of Fig. 3.2.1.6. They are analogous to the crystallographic groups. To facilitate the

use of the diagrams, the $(4N + 2)$-gonal and the $(2N + 1)$-gonal systems are combined, with the consequence that the five classes of the $(2N + 1)$-gonal system now appear with the symbols $\frac{1}{2}n\frac{2}{m}, \frac{1}{2}n2, \frac{1}{2}nm, \frac{1}{2}\bar{n}$ and $\frac{1}{2}n$. Again, the diagrams apply to a specified value of $N$. A finite number of further maximal subgroups is obtained for lower values of $N$, until the crystallographic groups (Fig. 3.2.1.3) are reached (*cf.* the two-dimensional examples in Fig. 3.2.1.5).

## 3.2.2. Point-group symmetry and physical properties of crystals

### By H. Klapper and Th. Hahn

In the previous section (Section 3.2.1), the crystallographic and noncrystallographic point groups are treated under geometrical aspects only. In the present section the point-group symmetries of the physical properties are considered. Among the physical properties, those represented by tensors are accessible to a mathematical treatment of their symmetries, which are apparent by the invariance of tensor components under symmetry operations. For more details the reader is referred to Nye (1957, 1985), Paufler (1986), Schwarzenbach & Chapuis (2006) and Shuvalov (1988). A similar comprehensive treatment of non-tensorial properties, such as cleavage, plasticity, hardness or crystal growth does not exist, but these properties are, of course, also governed by the crystallographic point-group symmetry.

### 3.2.2.1. General restrictions on physical properties imposed by symmetry

#### 3.2.2.1.1. Neumann's principle

Neumann's principle (Neumann, 1885) describes the relation between the symmetry $\mathcal{Q}$ of a physical property and the crystallographic point group $\mathcal{P}$ of a crystal. It states that the symmetry of any physical property of a crystal is higher than, or at least equal to, its crystallographic point-group symmetry, or in the language of groups, the symmetry $\mathcal{Q}$ of any physical property of a crystal is a proper or improper supergroup of its crystallographic symmetry $\mathcal{P}$: $\mathcal{Q} \subseteq \mathcal{P}$. This is easily illustrated for polar second-rank tensors, which are represented by ellipsoids and hyperboloids. The representation surfaces of triclinic, monoclinic and orthorhombic crystals are general ellipsoids or hyperboloids of symmetry $\mathcal{Q} = 2/m\,2/m\,2/m$, which is a proper supergroup of all triclinic, monoclinic and orthorhombic point groups with the only exception of the orthorhombic holohedry $\mathcal{P} = 2/m\,2/m\,2/m$, for which the two symmetries are the same. For the uniaxial crystals of the trigonal, tetragonal and hexagonal systems the representation ellipsoids and hyperboloids have rotation symmetries with the cylindrical point group $\mathcal{Q} = \infty/m\,2/m$ (see Table 3.2.1.6), which is a proper supergroup of all uniaxial crystallographic point groups. For cubic crystals, second-rank tensors are isotropic and represented by a sphere with point-group symmetry $\mathcal{Q} = 2/m\,\overline{\infty}$ ($\infty\infty m$), a proper supergroup of all cubic crystallographic point groups. For more details the reader is referred to Paufler (1986) and Authier (2014). A short resume is given by Klapper & Hahn (2005).

As a consequence of the invariance of tensor components under a symmetry operation (or alternatively: under a transformation of the coordinate system to a symmetry-equivalent one),

some of the tensor components are equal or even zero. The number of independent components decreases when the symmetry of the crystal increases. Thus, an increase of the point-group symmetry from 1 (triclinic) to $4/m\,\bar{3}\,2/m$ (cubic) or to the sphere group $\infty\infty m$ (*i.e.* isotropy) reduces the number of tensor components for symmetrical second-rank tensors from 6 to 1. Even more drastic is this reduction for all tensors of odd rank (such as pyroelectricity and piezoelectricity) or axial tensors of second rank (*e.g.* optical activity): all components are zero if an inversion centre is present, *i.e.* properties described by these tensors do not exist in centrosymmetric crystals (see the textbooks of tensor physics mentioned above). These properties, which exist only in noncentrosymmetric crystals are, as a rule, the most important ones, not only for physical applications but also for structure determination, because they allow a proof of the absence of a symmetry centre.

For the description of noncentrosymmetric crystals and their specific properties, certain notions are of importance and these are explained in the following two sections.

#### 3.2.2.1.2. Curie's principle

Curie's principle (Curie, 1894) describes the crystallographic symmetry $\mathcal{P}_F$ of a macroscopic crystal which is subject to an external influence $F$, for example to an electric field $\mathbf{E}$, to uniaxial stress $\sigma_{ii}$, to a temperature change $\Delta T$ *etc*. For this treatment, the point-group symmetries $\mathcal{R}$ of the external influences (Curie groups) are defined as follows (see Authier, 2014, p. 11; Paufler, 1986, p. 29):

Homogeneous electric field $\mathbf{E}$: $\mathcal{R} = \infty m$ (polar continuous rotation axis with 'parallel' mirror planes, *i.e.* symmetry of a stationary cone) [Note that a rotating cone (left- or right-handed) represents geometrically the polar enantiomorphous group $\infty$; a stationary cone represents the polar group $\infty m$ with 'vertical' mirror planes, *cf.* Section 3.2.1.4.1.];

Homogeneous magnetic field $\mathbf{H}$: $\mathcal{R} = \infty/m$ (symmetry of a rotating cylinder);

Uniaxial stress $\sigma_{ii}$: $\mathcal{R} = \infty/m\,2/m$ (symmetry of a stationary centrosymmetric cylinder);

Temperature change $\Delta T$ or hydrostatic pressure $p$ (scalars): $\mathcal{R} = 2/m\,\overline{\infty}$ ($\infty\infty m$) (symmetry of a stationary centrosymmetric sphere);

Shear stress $\sigma_{ij}$: $\mathcal{R} = 2/m\,2/m\,2/m$ (orthorhombic).

According to Curie's principle, the point-group symmetry $\mathcal{P}_F$ of the crystal under the external field $F$ is the intersection symmetry of the two point groups: $\mathcal{P}$ of the crystal without field and $\mathcal{R}$ of the field without crystal: $\mathcal{P}_F = \mathcal{R} \cap \mathcal{P}$; *i.e.* $\mathcal{P}_F$ is a (proper or improper) subgroup of both groups $\mathcal{R}$ and $\mathcal{P}$.

As examples we consider the effect of an electric field ($\mathcal{R} = \infty m$) and of a uniaxial stress ($\mathcal{R} = \infty/m\,2/m$) along one of the (four) threefold rotoinversion axes $\bar{3}$ of cubic crystals with point groups $\mathcal{P} = 2/m\,\bar{3}$ and $\mathcal{P} = 4/m\,\bar{3}\,2/m$.

Electric field parallel to [111]:

| | | |
|---|---|---|
| $2/m\,\bar{3} \cap \infty m$: | $\mathcal{P}_F = 3$ | along [111] (polar, pyroelectric, optically active; *cf.* Sections 3.2.2.5 and 3.2.2.4.2) |
| $4/m\,\bar{3}\,2/m \cap \infty m$: | $\mathcal{P}_F = 3m$ | along [111] (polar, pyroelectric, not optically active) |