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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		Hexagonal		Cubic	
n	1	C_1	2	C_2	4	C_4	3	C_3	6	C_6	23	T
$\bar{n}$	$\bar{1}$	C_i	$m \equiv \bar{2}$	C_s	$\bar{4}$	S_4	$\bar{3}$	C_{3i}	$\bar{6} \equiv 3/m$	C_{3h}	–	–
n/m			$2/m$	C_{2h}	$4/m$	C_{4h}	–	–	$6/m$	C_{6h}	$2/m\bar{3}$	T_h
$n22$			222	D_2	422	D_4	32	D_3	622	D_6	432	O
nmm			$mm2$	C_{2v}	$4mm$	C_{4v}	$3m$	C_{3v}	$6mm$	C_{6v}	–	–
$\bar{n}2m$			–	–	$\bar{4}2m$	D_{2d}	$\bar{3}2/m$	D_{3d}	$\bar{6}2m$	D_{3h}	$\bar{4}3m$	T_d
$n/m\,2/m\,2/m$			$2/m\,2/m\,2/m$	D_{2h}	$4/m\,2/m\,2/m$	D_{4h}	–	–	$6/m\,2/m\,2/m$	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 4*mm*.

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 {*hk*0}, {*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 {*hk*0} in point group 4 have face symmetry 1 and belong to the same general 'Wyckoff position' 4*b*, with Wyckoff letter *b*.

[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 {*h*0*l*} 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 {*h*0*l*} 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-

[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 $\bar{6}m2$ 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	∞m	$\boldsymbol{1(1)}$; $\boldsymbol{2(2)}$; $\boldsymbol{m(m)}$; $\boldsymbol{3(3)}$; $\boldsymbol{4(4)}$; $\boldsymbol{6(6)}$; $\boldsymbol{mm2(mm2)}$; $\boldsymbol{4mm(4mm)}$; $\boldsymbol{3m(3m)}$; $\boldsymbol{6mm(6mm)}$
2	Pinacoid or parallelohedron	Line segment through origin	2	$\frac{\infty}{m}m$	$\boldsymbol{\bar{1}(1)}$; $2(1)$; $m(1)$; $\boldsymbol{\frac{2}{m}(2, m)}$; $\boldsymbol{222(2.., .2., ..2)}$; $mm2(.m., m..)$; $\boldsymbol{mmm(2mm, m2m, mm2)}$; $\boldsymbol{\bar{4}(2..)}$; $\boldsymbol{\frac{4}{m}(4..)}$; $\boldsymbol{422(4..)}$; $\left\{\begin{matrix}\boldsymbol{\bar{4}2m(2.mm)}\\ \boldsymbol{\bar{4}m2(2mm.)}\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(4mm)}$; $\boldsymbol{\bar{3}(3)}$; $\left\{\begin{matrix}\boldsymbol{321(3..)}\\ \boldsymbol{312(3..)}\\ \boldsymbol{32\ (3.)}\end{matrix}\right.$; $\left\{\begin{matrix}\boldsymbol{\bar{3}m1(3m.)}\\ \boldsymbol{\bar{3}1m(3.m)}\\ \boldsymbol{\bar{3}m\ (3m)}\end{matrix}\right.$; $\boldsymbol{\bar{6}(3..)}$; $\boldsymbol{\frac{6}{m}(6..)}$; $\boldsymbol{622(6..)}$; $\left\{\begin{matrix}\boldsymbol{\bar{6}m2(3m.)}\\ \boldsymbol{\bar{6}2m(3.m)}\end{matrix}\right.$; $\boldsymbol{\frac{6}{m}mm(6mm)}$
3	Sphenoid, dome, or dihedron	Line segment	2	$mm2$	$\boldsymbol{2(1)}$; $\boldsymbol{m(1)}$; $\boldsymbol{mm2(.m., m..)}$
4	Rhombic disphenoid or rhombic tetrahedron	Rhombic tetrahedron	4	222	$\boldsymbol{222(1)}$
5	Rhombic pyramid	Rectangle	4	$mm2$	$\boldsymbol{mm2(1)}$
6	Rhombic prism	Rectangle through origin	4	mmm	$\boldsymbol{2/m(1)}$; $222(1)\dagger$; $mm2(1)$; $\boldsymbol{mmm(m.., .m., ..m)}$
7	Rhombic dipyramid	Rectangular prism	8	mmm	$\boldsymbol{mmm(1)}$
8	Tetragonal pyramid	Square	4	$4mm$	$\boldsymbol{4(1)}$; $\boldsymbol{4mm(..m, .m.)}$
9	Tetragonal disphenoid or tetragonal tetrahedron	Tetragonal tetrahedron	4	$\bar{4}2m$	$\boldsymbol{\bar{4}(1)}$; $\left\{\begin{matrix}\boldsymbol{\bar{4}2m(..m)}\\ \boldsymbol{\bar{4}m2(.m.)}\end{matrix}\right.$
10	Tetragonal prism	Square through origin	4	$\frac{4}{m}mm$	$4(1)$; $\bar{4}(1)$; $\boldsymbol{\frac{4}{m}(m..)}$; $\boldsymbol{422(..2, .2.)}$; $4mm(..m, .m.)$; ‡ $\left\{\begin{matrix}\boldsymbol{\bar{4}2m(.2.)} \text{ and } \bar{4}2m(..m)\\ \boldsymbol{\bar{4}m2(..2)} \text{ and } \bar{4}m2(.m.)\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(m.m2, m2m.)}$
11	Tetragonal trapezohedron	Twisted tetragonal antiprism	8	422	$\boldsymbol{422(1)}$
12	Ditetragonal pyramid	Truncated square	8	$4mm$	$\boldsymbol{4mm(1)}$
13	Tetragonal scalenohedron	Tetragonal tetrahedron cut off by pinacoid	8	$\bar{4}2m$	$\left\{\begin{matrix}\boldsymbol{\bar{4}2m(1)}\\ \boldsymbol{\bar{4}m2(1)}\end{matrix}\right.$
14	Tetragonal dipyramid	Tetragonal prism	8	$\frac{4}{m}mm$	$\boldsymbol{\frac{4}{m}(1)}$; $422(1)\dagger$; $\left\{\begin{matrix}\bar{4}2m(1)\\ \bar{4}m2(1)\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(.m, .m.)}$
15	Ditetragonal prism	Truncated square through origin	8	$\frac{4}{m}mm$	$422(1)$; $4mm(1)$; $\left\{\begin{matrix}\bar{4}2m(1)\\ \bar{4}m2(1)\end{matrix}\right.$; $\boldsymbol{\frac{4}{m}mm(m..)}$
16	Ditetragonal dipyramid	Edge-truncated tetragonal prism	16	$\frac{4}{m}mm$	$\boldsymbol{\frac{4}{m}mm(1)}$
17	Trigonal pyramid	Trigon	3	$3m$	$\boldsymbol{3(1)}$; $\left\{\begin{matrix}\boldsymbol{3m1(.m.)}\\ \boldsymbol{31m(..m)}\\ \boldsymbol{3m\ (.m)}\end{matrix}\right.$

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	$\bar{6}2m$	3(1); { **321(.2.)** **312(..2)** **32 (.2)** }; { 3*m*1(.*m*.) 31*m*(..*m*) 3*m* (.*m*) }; **$\bar{6}$(*m*..)**; { **$\bar{6}$*m*2(*mm*2)** **$\bar{6}$2*m*(*m*2*m*)** }
19	Trigonal trapezohedron	Twisted trigonal antiprism	6	32	{ **321(1)** **312(1)** **32 (1)** }
20	Ditrigonal pyramid	Truncated trigon	6	$3m$	{ **3*m*1(1)** **31*m*(1)** **3*m* (1)** }
21	Rhombohedron	Trigonal antiprism	6	$\bar{3}m$	**$\bar{3}$(1)**; { 321(1) 312(1) 32 (1) }; { **$\bar{3}$*m*1(.*m*.)** **$\bar{3}$1*m*(..*m*)** **$\bar{3}$*m* (.*m*)** }
22	Ditrigonal prism	Truncated trigon through origin	6	$\bar{6}2m$	{ 321(1) 312(1) 32 (1) }; { 3*m*1(1) 31*m*(1) 3*m* (1) }; { **$\bar{6}$*m*2(*m*..)** **$\bar{6}$2*m*(*m*..)** }
23	Hexagonal pyramid	Hexagon	6	$6mm$	{ 3*m*1(1) 31*m*(1) 3*m* (1) }; **6(1)**; **6*mm*(..*m*, .*m*.)**
24	Trigonal dipyramid	Trigonal prism	6	$\bar{6}2m$	{ 321(1) 312(1) 32 (1) }; **$\bar{6}$(1)**; { **$\bar{6}$*m*2(.*m*.)** **$\bar{6}$2*m*(..*m*)** }
25	Hexagonal prism	Hexagon through origin	6	$\frac{6}{m}mm$	$\bar{3}$(1); { 321(1) 312(1) 32 (1) }; { 3*m*1(1) 31*m*(1) 3*m* (1) } ‡ { **$\bar{3}$*m*1(.2.)** and $\bar{3}$*m*1(.*m*.) **$\bar{3}$1*m*(..2)** and $\bar{3}$1*m*(..*m*) **$\bar{3}$*m*(.2)** and $\bar{3}$*m*(.*m*) }; 6(1); **$\frac{6}{m}$(*m*..)**; **622(.2., ..2)**; 6*mm*(..*m*, .*m*.); { $\bar{6}$*m*2(*m*..) $\bar{6}$2*m*(*m*..) }; **$\frac{6}{m}$*mm*(*m*2*m*, *mm*2)**
26	Ditrigonal scalenohedron or hexagonal scalenohedron	Trigonal antiprism sliced off by pinacoid	12	$\bar{3}m$	{ **$\bar{3}$*m*1(1)** **$\bar{3}$1*m*(1)** **$\bar{3}$*m* (1)** }
27	Hexagonal trapezohedron	Twisted hexagonal antiprism	12	622	**622(1)**
28	Dihexagonal pyramid	Truncated hexagon	12	$6mm$	**6*mm*(1)**
29	Ditrigonal dipyramid	Edge-truncated trigonal prism	12	$\bar{6}2m$	{ **$\bar{6}$*m*2(1)** **$\bar{6}$2*m*(1)** }
30	Dihexagonal prism	Truncated hexagon	12	$\frac{6}{m}mm$	{ $\bar{3}$*m*1(1) $\bar{3}$1*m*(1) $\bar{3}$*m* (1) }; 622(1); 6*mm*(1); **$\frac{6}{m}$*mm*(*m*..)**
31	Hexagonal dipyramid	Hexagonal prism	12	$\frac{6}{m}mm$	{ $\bar{3}$*m*1(1) $\bar{3}$1*m*(1) $\bar{3}$*m* (1) }; $\frac{6}{m}$(1); 622(1)†; { $\bar{6}$*m*2(1) $\bar{6}$2*m*(1) }; **$\frac{6}{m}$*mm*(..*m*, .*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	$\frac{6}{m}mm$	$\boldsymbol{\frac{6}{m}mm(1)}$
33	Tetrahedron	Tetrahedron	4	$\bar{4}3m$	$\mathbf{23(.3.)}$; $\boldsymbol{\bar{4}3m(.3m)}$
34	Cube or hexahedron	Octahedron	6	$m\bar{3}m$	$\mathbf{23(2..)}$; $\boldsymbol{m\bar{3}(2mm..)}$; $\mathbf{432(4..)}$; $\boldsymbol{\bar{4}3m(2.mm)}$; $\boldsymbol{m\bar{3}m(4m.m)}$
35	Octahedron	Cube	8	$m\bar{3}m$	$\boldsymbol{m\bar{3}(.3.)}$; $\mathbf{432(.3.)}$; $\boldsymbol{m\bar{3}m(.3m)}$
36	Pentagon-tritetrahedron or tetartoid or tetrahedral pentagon-dodecahedron	Snub tetrahedron (= pentagon-tritetrahedron + two tetrahedra)	12	23	$\mathbf{23(1)}$
37	Pentagon-dodecahedron or dihexahedron or pyritohedron	Irregular icosahedron (= pentagon-dodecahedron + octahedron)	12	$m\bar{3}$	23(1); $\boldsymbol{m\bar{3}(m..)}$
38	Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron	Cube and two tetrahedra	12	$\bar{4}3m$	23(1); $\boldsymbol{\bar{4}3m(..m)}$
39	Trigon-tritetrahedron or tristetrahedron	Tetrahedron truncated by tetrahedron	12	$\bar{4}3m$	23(1); $\boldsymbol{\bar{4}3m(..m)}$
40	Rhomb-dodecahedron	Cuboctahedron	12	$m\bar{3}m$	23(1); $m\bar{3}(m..)$; $\mathbf{432(..2)}$; $\bar{4}3m(..m)$; $\boldsymbol{m\bar{3}m(m.m2)}$
41	Didodecahedron or diploid or dyakisdodecahedron	Cube & octahedron & pentagon-dodecahedron	24	$m\bar{3}$	$\boldsymbol{m\bar{3}(1)}$
42	Trigon-trioctahedron or trisoctahedron	Cube truncated by octahedron	24	$m\bar{3}m$	$m\bar{3}(1)$; 432(1); $\boldsymbol{m\bar{3}m(..m)}$
43	Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron	Cube & octahedron & rhomb-dodecahedron	24	$m\bar{3}m$	$m\bar{3}(1)$; 432(1); $\boldsymbol{m\bar{3}m(..m)}$
44	Pentagon-trioctahedron or gyroid	Cube + octahedron + pentagon-trioctahedron	24	432	$\mathbf{432(1)}$
45	Hexatetrahedron or hexakistetrahedron	Cube truncated by two tetrahedra	24	$\bar{4}3m$	$\boldsymbol{\bar{4}3m(1)}$
46	Tetrahexahedron or tetrakishexahedron	Octahedron truncated by cube	24	$m\bar{3}m$	432(1); $\bar{4}3m(1)$; $\boldsymbol{m\bar{3}m(m..)}$
47	Hexaoctahedron or hexakisoctahedron	Cube truncated by octahedron and by rhomb-dodecahedron	48	$m\bar{3}m$	$\boldsymbol{m\bar{3}m(1)}$

† 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 '$\boldsymbol{\bar{4}2m(.2.)}$ and $\bar{4}2m(..m)$' and as '$\boldsymbol{\bar{3}m1(.2.)}$ 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

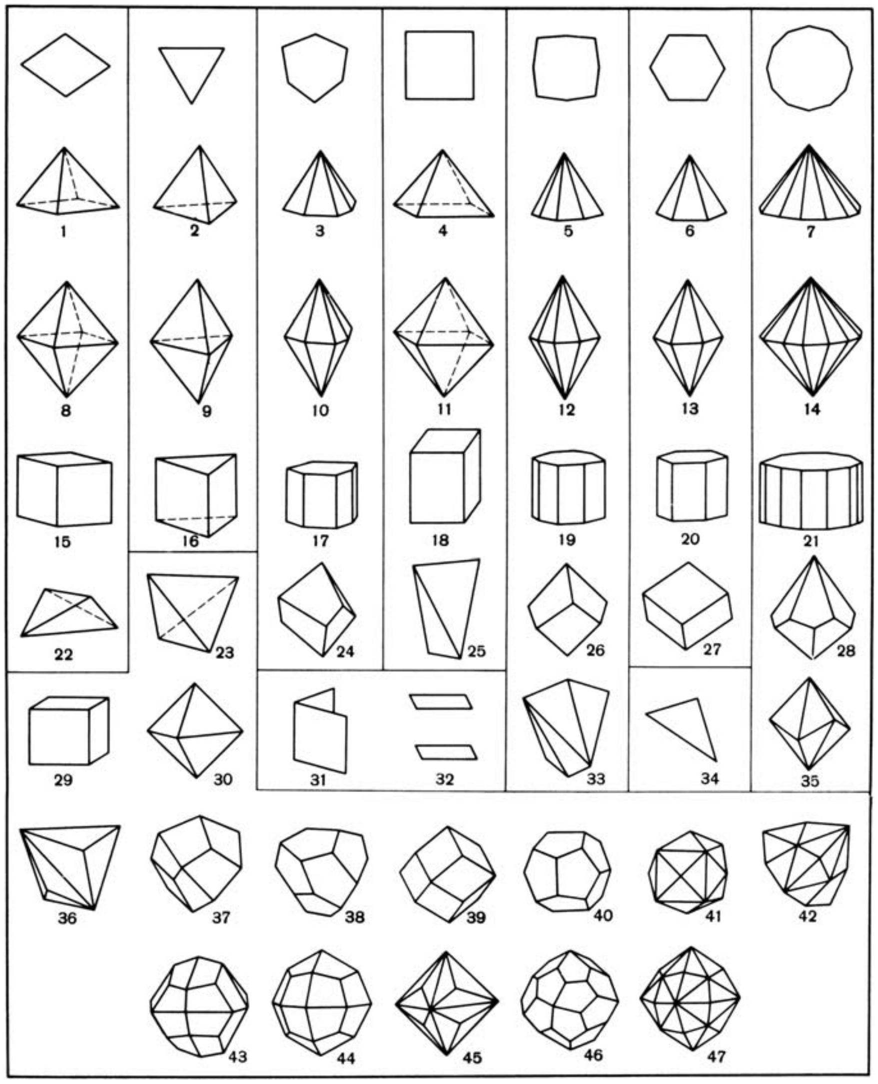


Figure 3.2.1.1
The 47 crystal forms that crystals may take (from Shubnikov & Koptsik, 1974, p. 74): (1)–(7) Pyramids: orthorhombic, trigonal, ditrigonal, tetragonal, ditetragonal, hexagonal, dihexagonal; (8)–(14) bipyramids of the same types; (15)–(21) prisms of the same types; (22), (23), (25) tetrahedra: 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

[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: International symbol: Short	Full	Schoenflies symbol	Class names: Groth (1921)	Friedel (1926)	
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	
	$2/m$	$\frac{2}{m}$	C_{2h}	Prismatic	Holohedry	
Orthorhombic	222	222	$D_2(V)$	Disphenoidal	Holoaxial hemihedry	
	$mm2$	$mm2$	C_{2v}	Pyramidal	Antihemihedry	
	mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_{2h}(V_h)$	Dipyramidal	Holohedry	
Tetragonal	4	4	C_4	Pyramidal	Tetartohedry with 4-axis	
	$\bar{4}$	$\bar{4}$	S_4	Disphenoidal	Sphenohedral tetartohedry	
	$4/m$	$\frac{4}{m}$	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	
	$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	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
	$\bar{3}m$	$\bar{3}\frac{2}{m}$	D_{3d}	Ditrigonal-scalenohedral	Parahemihedry with 3-axis	Holohedry
Hexagonal	6	6	C_6	Pyramidal	Tetartohedry with 6-axis	
	$\bar{6}$	$\bar{6}$	C_{3h}	Trigonal-dipyramidal	Trigonohedral antitetartohedry	
	$6/m$	$\frac{6}{m}$	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	
	$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	D_{6h}	Dihexagonal-dipyramidal	Holohedry	
Cubic	23	23	T	Tetrahedral-pentagondodecahedral (= tetartoidal)	Tetartohedry	
	$m\bar{3}$	$\frac{2}{m}\bar{3}$	T_h	Disdodecahedral (= diploidal)	Parahemihedry	
	432	432	O	Pentagon-icositetrahedral (= gyroidal)	Holoaxial hemihedry	
	$\bar{4}3m$	$\bar{4}3m$	T_d	Hexakistetrahedral (= hextetrahedral)	Antihemihedry	
	$m\bar{3}m$	$\frac{4}{m}\bar{3}\frac{2}{m}$	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 $\bar{4}$, the general crystal form 4*b* is listed as (hkl) $(\bar{h}\bar{k}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$: the corresponding general position 4*h* of the symmorphic space group $P\bar{4}$ reads x, y, z; $\bar{x}, \bar{y}, z$; $y, \bar{x}, \bar{z}$; $\bar{y}, x, \bar{z}$.

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

(3) The Miller indices of the *cubic point groups* are arranged in one, two or four blocks of (3×4) entries. The first block belongs to point group 23. The second block belongs to the diagonal twofold axes in 432 and $m\bar{3}m$ or to the diagonal mirror plane in $\bar{4}3m$. In point groups $m\bar{3}$ and $m\bar{3}m$, 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 $\{10\bar{1}0\}$ 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 $(00\bar{1})$;

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

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

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

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

(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 *semi-regular* 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

[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 χ. The trapezohedron changes into the limiting forms 'trigonal dipyramid' $\{hhl\}$ for $\chi = 0^\circ$ and 'rhombohedron' $\{h0l\}$ for $\chi = 60^\circ$.

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

Examples

(1) A tetragonal 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 $\bar{4}2m$.
(2) A tetragonal prism appears in point group $\bar{4}2m$ 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 $m\bar{3}m$ and $\bar{4}3m$, the two kinds of polyhedra represent two realizations of one *special* 'Wyckoff position'; hence, they have the same Wyckoff letter. In the groups 23, $m\bar{3}$ and 432, they represent two realizations of the same type of limiting *general* forms. In the tables of the cubic point groups, the two entries are always connected by braces.

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

3.2.1.2.5. Names and symbols of the crystal classes

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

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

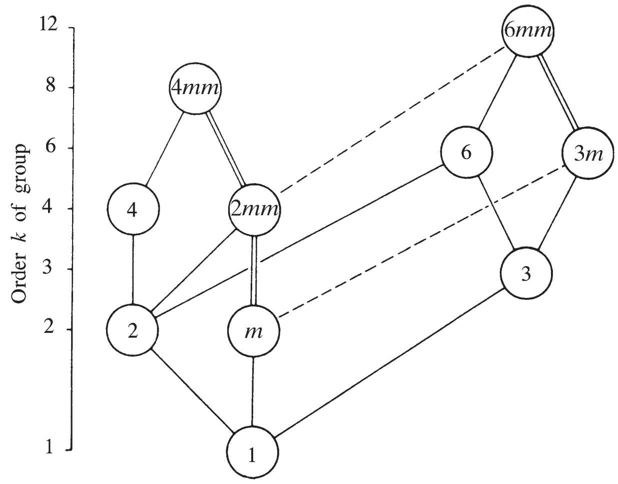


Figure 3.2.1.2
Maximal subgroups and minimal supergroups of the two-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left.

or rhombohedral: *e.g.* 'hexagonal ogdohedry' and 'rhombohedral tetartohedry'.

3.2.1.3. Subgroups and supergroups of the crystallographic point groups

In this section, the sub- and supergroup relations between the crystallographic point groups are presented in the form of a 'family tree'.[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

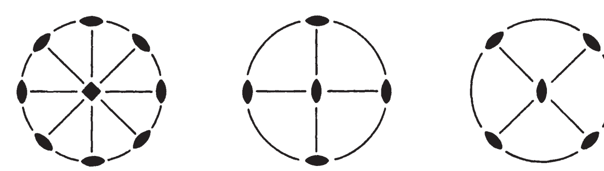
(1) Point group $3m$ has three different mirror planes which are equivalent due to the threefold axis. In each of the three maximal subgroups of type m, one of these mirror planes is retained. Hence, the three subgroups m are conjugate in $3m$. This set of conjugate subgroups is represented by *one*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

(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.



422 222. 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.

[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.