

## 3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

Face poles marked as dots lie above the projection plane and represent faces which intersect the positive  $c$  axis<sup>2</sup> (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.<sup>3</sup>

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’ 4b, with Wyckoff letter b.

<sup>2</sup> 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.

<sup>3</sup> Dual polyhedra have the same number of edges, but the numbers of faces and vertices are interchanged; cf. textbooks of geometry.

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- (2) All tetragonal pyramids *and* tetragonal prisms in point group  $4mm$  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  $4c$ ; for the oriented face symmetry  $..m$ , the forms  $\{hhl\}$  and  $\{110\}$  belong to Wyckoff position  $4b$ . The face symmetries  $.m.$  and  $..m$  are not conjugate in point group  $4mm$ . 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  $4b$  in point group  $4$  has generating symmetry  $4$  and eigensymmetry  $4mm$ ; each tetragonal prism  $\{hk0\}$  of the same Wyckoff position has generating symmetry  $4$  again, but eigensymmetry  $4/mmm$ .
- (2) A cube  $\{100\}$  may have generating symmetry  $23, m\bar{3}, 432, \bar{4}3m$  or  $m\bar{3}m$ , but its eigensymmetry is always  $m\bar{3}m$ .

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  $4mm$ ;
- (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’)  $1, 2, 3, 4, 6, \bar{1}, m, \bar{3}, \bar{4}, \bar{6} = 3/m, 2/m, 4/m, 6/m$  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).<sup>4</sup>

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<sup>5</sup> 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<sup>6</sup> 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  $4mm$  are basic forms of the general Wyckoff position  $4b$ , whereas the forms  $\{hk0\}$  (tetragonal prisms) of higher eigensymmetry  $4/mmm$  are ‘limiting general forms’. The face poles of forms  $\{hk0\}$  lie on the horizontal mirror plane of the supergroup  $4/m$ .
- (2) In point group  $4mm$ , the (characteristic) special crystal forms  $\{h0l\}$  with eigensymmetry  $4mm$  are ‘basic forms’ of the special Wyckoff position  $4c$ , 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  $4mm$  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-

<sup>4</sup> 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.

<sup>5</sup> 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).

<sup>6</sup> 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.

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

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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	$\bar{6}2m$	$3(1); \left\{ \begin{array}{l} 321(.2) \\ 312(..2) \\ 32 (.2) \end{array} \right\}; \left\{ \begin{array}{l} 3m1(.m.) \\ 31m(..m) \\ 3m (.m) \end{array} \right\};$ $\bar{6}(m.); \left\{ \begin{array}{l} \bar{6}m2(mm2) \\ \bar{6}2m(m2m) \end{array} \right\}$
19	Trigonal trapezohedron	Twisted trigonal antiprism	6	32	$\left\{ \begin{array}{l} 321(1) \\ 312(1) \\ 32 (1) \end{array} \right\}$
20	Ditrigonal pyramid	Truncated trigon	6	3m	$\left\{ \begin{array}{l} 3m1(1) \\ 31m(1) \\ 3m (1) \end{array} \right\}$
21	Rhombohedron	Trigonal antiprism	6	$\bar{3}m$	$\bar{3}(1); \left\{ \begin{array}{l} 321(1) \\ 312(1) \\ 32 (1) \end{array} \right\}; \left\{ \begin{array}{l} \bar{3}m1(.m.) \\ \bar{3}1m(..m) \\ \bar{3}m (.m) \end{array} \right\}$
22	Ditrigonal prism	Truncated trigon through origin	6	$\bar{6}2m$	$\left\{ \begin{array}{l} 321(1) \\ 312(1) \\ 32 (1) \end{array} \right\}; \left\{ \begin{array}{l} 3m1(1) \\ 31m(1) \\ 3m (1) \end{array} \right\};$ $\left\{ \begin{array}{l} \bar{6}m2(m..) \\ \bar{6}2m(m..) \end{array} \right\}$
23	Hexagonal pyramid	Hexagon	6	6mm	$\left\{ \begin{array}{l} 3m1(1) \\ 31m(1); 6(1); 6mm(..m, .m.) \\ 3m (1) \end{array} \right\}$
24	Trigonal dipyramid	Trigonal prism	6	$\bar{6}2m$	$\left\{ \begin{array}{l} 321(1) \\ 312(1); \bar{6}(1); \left\{ \begin{array}{l} \bar{6}m2(.m.) \\ \bar{6}2m(..m) \end{array} \right\} \\ 32 (1) \end{array} \right\}$
25	Hexagonal prism	Hexagon through origin	6	$\frac{6}{m}mm$	$\bar{3}(1); \left\{ \begin{array}{l} 321(1) \\ 312(1) \\ 32 (1) \end{array} \right\}; \left\{ \begin{array}{l} 3m1(1) \\ 31m(1) \\ 3m (1) \end{array} \right\};$ $\ddagger \left\{ \begin{array}{l} \bar{3}m1(.2) \text{ and } \bar{3}m1(.m.) \\ \bar{3}1m(..2) \text{ and } \bar{3}1m(..m) \\ \bar{3}m(.2) \text{ and } \bar{3}m(.m) \end{array} \right\};$ $6(1); \frac{6}{m}(m.); 622(.2., ..2);$ $6mm(..m, .m.); \left\{ \begin{array}{l} \bar{6}m2(m..) \\ \bar{6}2m(m..) \end{array} \right\};$ $\frac{6}{m}mm(m2m, mm2)$
26	Ditrigonal scalenohedron or hexagonal scalenohedron	Trigonal antiprism sliced off by pinacoid	12	$\bar{3}m$	$\left\{ \begin{array}{l} \bar{3}m1(1) \\ \bar{3}1m(1) \\ \bar{3}m (1) \end{array} \right\}$
27	Hexagonal trapezohedron	Twisted hexagonal antiprism	12	622	622(1)
28	Dihexagonal pyramid	Truncated hexagon	12	6mm	6mm(1)
29	Ditrigonal dipyramid	Edge-truncated trigonal prism	12	$\bar{6}2m$	$\left\{ \begin{array}{l} \bar{6}m2(1) \\ \bar{6}2m(1) \end{array} \right\}$
30	Dihexagonal prism	Truncated hexagon	12	$\frac{6}{m}mm$	$\left\{ \begin{array}{l} \bar{3}m1(1) \\ \bar{3}1m(1); 622(1); 6mm(1); \\ \bar{3}m (1) \end{array} \right\};$ $\frac{6}{m}mm(m..)$
31	Hexagonal dipyramid	Hexagonal prism	12	$\frac{6}{m}mm$	$\left\{ \begin{array}{l} \bar{3}m1(1) \\ \bar{3}1m(1); \frac{6}{m}(1); 622(1)\ddagger; \\ \bar{3}m (1) \end{array} \right\};$ $\left\{ \begin{array}{l} \bar{6}m2(1); \frac{6}{m}mm(..m, .m.) \\ \bar{6}2m(1) \end{array} \right\};$

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**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 tetrakisohedron	Octahedron truncated by cube	24	$m\bar{3}m$	$432(1); \bar{4}3m(1); m\bar{3}m(m.)$
47	Hexaoctahedron or hexakisohedron	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 ' $\bar{3}m(2.)$ ' and ' $\bar{3}m(m.)$ '.

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*

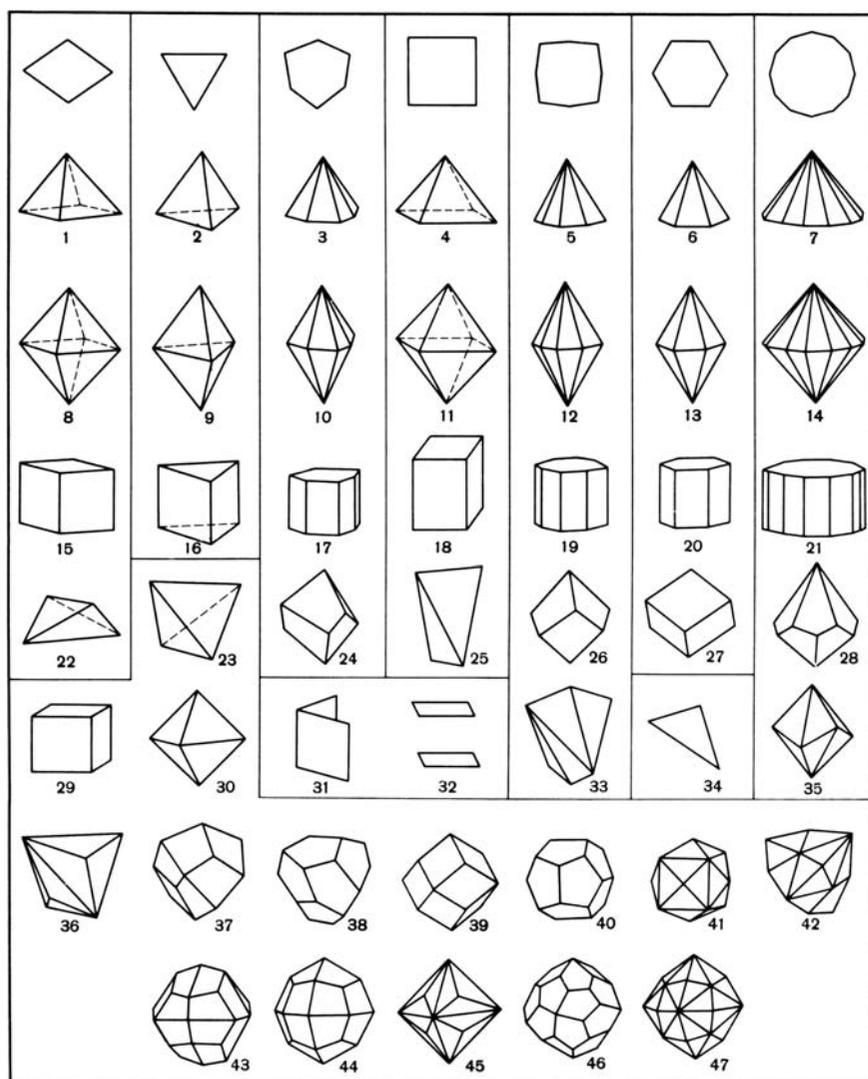
- (1) In point group 32, the limiting general crystal forms are of four types:
  - (i) ditrigonal prisms, eigensymmetry  $\bar{6}2m$  (face poles on horizontal mirror plane of holohedry  $6/mmm$ );
  - (ii) trigonal dipyramids, eigensymmetry  $\bar{6}2m$  (face poles on one kind of vertical mirror plane);

- (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

### 3.2. POINT GROUPS AND CRYSTAL CLASSES



**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,<sup>7</sup> 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

<sup>7</sup> For the exceptions in the cubic crystal system *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).