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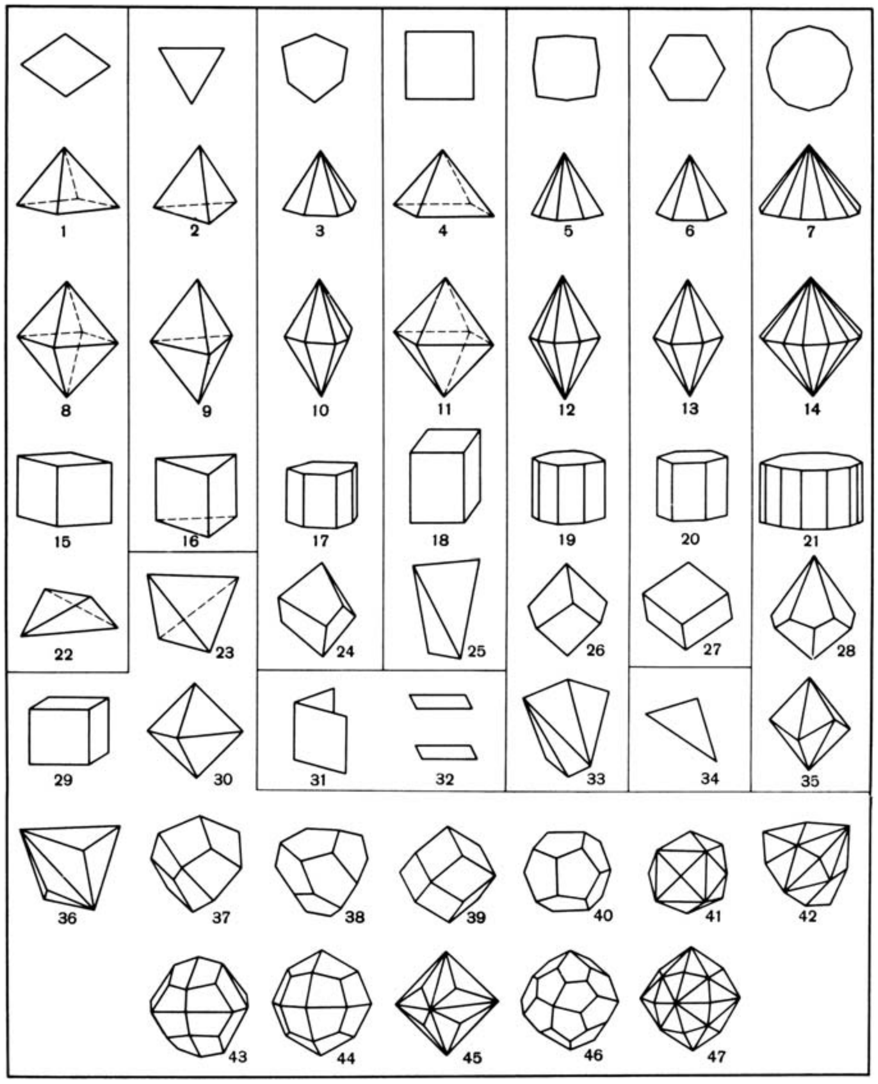

Figure 3.2.1.1
The 47 crystal forms that crystals may take (from Shubnikov & Koptsik, 1974, p. 74): (1)–(7) Pyramids: orthorhombic, trigonal, ditrigonal, tetragonal, ditetragonal, hexagonal, dihexagonal; (8)–(14) bipyramids of the same types; (15)–(21) prisms of the same types; (22), (23), (25) tetrahedra: 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	Point group: International symbol: Full	Schoenflies symbol	Class names: Groth (1921)	Class names: 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 $4b$ is listed as (hkl) $(\bar{h}\bar{k}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$: the corresponding general position $4h$ 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 $3b$ is listed as $(hkil)$ $(ihkl)$ $(kihl)$ with $i = -(h + k)$; the corresponding general point form $3b$ 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}.