*International Tables for Crystallography* (2016). Vol. A, Section 3.2.1.2.4, pp. 729–730.



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 $(3 \times 4)$ 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 $\chi$. The trapezohedron changes into the limiting forms 'trigonal dipyramid' $\{hhl\}$ for $\chi = 0°$ and 'rhombohedron' $\{h0l\}$ for $\chi = 60°$.

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

*Examples*

(1) A tetragonal dipyramid is a general form in point group $4/m$, a special form in point group $4/mmm$ and a limiting general form in point groups 422 and $\bar{4}2m$.
(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