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Table 10.1.1.2. *The 32 three-dimensional crystallographic point groups, arranged according to crystal system (cf. Chapter 2.1)*

Full Hermann–Mauguin (left) and Schoenflies symbols (right). Dashed lines separate point groups with different Laue classes within one crystal system.

| 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 | $O$ |
| $nmm$ | | | $mm2$ | $C_{2v}$ | $4mm$ | $C_{4v}$ | $3m$ | $C_{3v}$ | $6mm$ | $C_{6v}$ | – | – |
| $\bar{n}2m$ | | | – | – | $\bar{4}2m$ | $D_{2d}$ | $\bar{3}2/m$ | $D_{3d}$ | $\bar{6}2m$ | $D_{3h}$ | $\bar{4}3m$ | $T_d$ |
| $n/m\,2/m\,2/m$ | | | $2/m\,2/m\,2/m$ | $D_{2h}$ | $4/m\,2/m\,2/m$ | $D_{4h}$ | – | – | $6/m\,2/m\,2/m$ | $D_{6h}$ | $4/m\,\bar{3}\,2/m$ | $O_h$ |

## 10.1.2. Crystallographic point groups

### 10.1.2.1. *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; this also applies to the construction and the properties of the stereographic projection.

In Tables 10.1.2.1 and 10.1.2.2, 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 10.1.2.1 and 10.1.2.2, some point groups are described in *two or three versions*, in order to bring out the relations to the corresponding space groups (*cf.* Section 2.2.3):

(*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 7. 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 Section 2.2.4 and Chapter 12.1.

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 2.1.2.1 and illustrated in Figs. 2.2.6.1 to 2.2.6.10.

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 1.4. 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* (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.†

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 under *Crystal and point forms*; the explanation of the listed data is to be found under *Description of crystal and point forms.*

* 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. 2.2.6.9.

† Dual polyhedra have the same number of edges, but the numbers of faces and vertices are interchanged; *cf.* textbooks of geometry.

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 2.2.14. 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*.

### 10.1.2.2. *Crystal and point forms*

For a point group $\mathcal{P}$ a *crystal form* is a set of all symmetrically equivalent faces; a *point form* is a set of all symmetrically equivalent points. Crystal and point forms in point groups correspond to 'crystallographic orbits' in space groups; *cf.* Section 8.3.2.

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 symmetrically 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 symmetrically 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 symmetrically 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 symmetrically 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 $x, y, 0$; $x, x, z$; $x, 0, 0$. The point $0, 0, 0$ is not considered to be a point form.

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 and point 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 2.2.11 and 8.3.2. In point groups, the term 'position' can be visualized as the position of the face poles and points in the stereographic projection. Each 'Wyckoff position' is labelled by a *Wyckoff letter*.

*Definition*

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

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

*Examples*

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

(2) All tetragonal pyramids *and* tetragonal prisms in point group 4*mm* belong to two special 'Wyckoff positions', depending on the orientation of their face-symmetry groups *m* with respect to the crystal axes: For the 'oriented face symmetry' *.m.*, the forms $\{h0l\}$ and $\{100\}$ belong to Wyckoff position 4*c*; for the oriented face symmetry *..m*, the forms $\{hhl\}$ and $\{110\}$ belong to Wyckoff position 4*b*. The face symmetries *.m.* and *..m* are not conjugate in point group 4*mm*. For the analogous 'oriented site symmetries' in space groups, see Section 2.2.12.

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* $\mathcal{C}$. The *eigensymmetry point group* $\mathcal{C}$ 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*



references