3.2. Point groups and crystal classes

Th. Hahn, H. Klapper, U. Müller and M. I. Aroyo

3.2.1. Crystallographic and noncrystallographic point groups

By Th. Hahn and H. Klapper

3.2.1.1. Introduction and definitions

A *point group*[1] is a group of symmetry operations all of which leave at least one point unmoved. Thus, all operations containing translations are excluded. Point groups can be subdivided into crystallographic and noncrystallographic point groups. A *crystallographic* point group is a point group that maps a point lattice onto itself. Consequently, rotations and rotoinversions are restricted to the well known crystallographic cases 1, 2, 3, 4, 6 and $\overline{1}$, $\overline{2} = m$, $\overline{3}$, $\overline{4}$, $\overline{6}$ (*cf.* Section 1.2.1); matrices for these symmetry operations are listed in Tables 1.2.2.1 and 1.2.2.2. No such restrictions apply to the *noncrystallographic* point groups.

The numbers of the crystallographic point groups are finite: 2 for one dimension, 10 for two dimensions and 32 for three dimensions. The numbers of noncrystallographic point groups for dimensions $n \geq 2$ are infinite. The two- and three-dimensional crystallographic point groups and their crystal systems are summarized in Tables 3.2.1.1 and 3.2.1.2. They are described in detail in Section 3.2.1.2. The two one-dimensional point groups are discussed in Section 2.1.3.16. The noncrystallographic point groups are treated in Section 3.2.1.4.

Crystallographic point groups occur:

(i) in vector space as symmetries of the external shapes of crystals, *i.e.* of the set of vectors normal to the crystal faces (morphological symmetry); this also includes the symmetries of sets of symmetry-equivalent net planes in crystals (reciprocal-lattice points), fundamental for the theory of X-ray diffraction.

(ii) in point space as site symmetries of points in lattices or in crystal structures and as symmetries of molecules, atomic groups and coordination polyhedra.

General point groups, *i.e.* crystallographic *and* noncrystallographic point groups, occur as:

(iii) symmetries of (rigid) molecules (molecular symmetry):

(iv) symmetries of physical properties of crystals (*e.g.* tensor symmetries); here noncrystallographic point groups with axes of order infinity are of particular importance, as in the symmetries of circles, spheres or rotation ellipsoids:

(v) approximate symmetries of the local environment of a point in a crystal structure, *i.e.* as *local* site symmetries. Examples are sphere-like atoms or ions in crystals, as well as icosahedral atomic groups. These noncrystallographic symmetries, however, are only approximate, even for the close neighbourhood of a site.

A (geometric) *crystal class* (point-group type) is the set of all crystals having the same point-group symmetry. The word 'class', therefore, denotes a classificatory pigeonhole and should not be used as synonymous with the point group of a particular crystal. The symbol of a crystal class is that of the common point group. (For geometric and arithmetic crystal classes of space groups, see Sections 1.3.4.2 and 1.3.4.4.)

Of particular importance for the structure determination of crystals are the 11 *centrosymmetric crystallographic point groups*, because they describe the possible symmetries of the diffraction record of a crystal: $\overline{1}$; $2/m$; mmm; $4/m$; $4/mmm$; $\overline{3}$; $\overline{3}m$; $6/m$; $6/mmm$; $m\overline{3}$; $m\overline{3}m$. This is due to Friedel's rule, which states that, provided anomalous dispersion is neglected, the diffraction record of any crystal is centrosymmetric, even if the crystal is noncentrosymmetric. The symmetry of the diffraction record determines the *Laue class* of the crystal; this is further explained in Chapter 1.6. For a given crystal, its Laue class is obtained if a symmetry centre is added to its point group, as shown in Table 3.2.2.1.

In two dimensions, six 'centrosymmetric' crystallographic point groups and hence six two-dimensional Laue classes exist: 2; 2*mm*; 4; 4*mm*; 6; 6*mm*. These point groups are, for instance, the only possible symmetries of zero-layer X-ray photographs.

Among the centrosymmetric crystallographic point groups in three dimensions, the seven *lattice point groups* (holohedral point groups, *holohedries*) are of special importance because they constitute the possible point symmetries of lattices, *i.e.* the site symmetries of their nodes. In three dimensions, the seven holohedries are: $\overline{1}$; $2/m$; mmm; $4/mmm$; $\overline{3}m$; $6/mmm$; $m\overline{3}m$. Note that $\overline{3}m$ is the point symmetry of the rhombohedral lattice and $6/mmm$ the point symmetry of the hexagonal lattice; both occur in the hexagonal crystal family (*cf.* Chapter 2.1). Point groups that are, within a crystal family, subgroups of a holohedry are called merohedries; they are called specifically hemihedries for subgroups of index 2, tetartohedries for index 4 and ogdohedries for index 8.

In two dimensions, four holohedries exist: 2; 2*mm*; 4*mm*; 6*mm*. Note that the hexagonal crystal family in two dimensions contains only one lattice type, with point symmetry 6*mm*.

Another classification of the crystallographic point groups is that into isomorphism classes. Here all those point groups that have the same kind of group table appear in one class. These isomorphism classes are also known under the name of *abstract point groups*.

There are 18 abstract crystallographic point groups in three dimensions: the point groups in each of the following lines are isomorphous and belong to the same abstract group:

Table 3.2.1.1
The ten two-dimensional crystallographic point groups, arranged according to crystal system

The dashed line separates point groups with different Laue classes within one crystal system.

General symbol	Crystal system				
	Oblique (top) Rectangular (bottom)		Square	Hexagonal	
n	1	2	4	3	6
nmm	m	2*mm*	4*mm*	3*m*	6*mm*

[1] For reasons of simplicity, in this chapter the same term 'point group' is used for a 'particular point group' *and* a 'type of point group'. For space groups, this distinction is explained in Section 1.3.4.1. For a different use of the term 'point group' see Section 1.3.3.1.

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
$\overline{n}$	$\overline{1}$	C_i	$m \equiv \overline{2}$	C_s	$\overline{4}$	S_4	$\overline{3}$	C_{3i}	$\overline{6} \equiv 3/m$	C_{3h}	–	–
n/m			$2/m$	C_{2h}	$4/m$	C_{4h}	–	–	$6/m$	C_{6h}	$2/m\overline{3}$	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}	–	–
$\overline{n}2m$			–	–	$\overline{4}2m$	D_{2d}	$\overline{3}2/m$	D_{3d}	$\overline{6}2m$	D_{3h}	$\overline{4}3m$	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}	$4/m\,\overline{3}\,2/m$	O_h

Order 1: 1
2: $\overline{1}$, 2, m
3: 3
4: $2/m$, 222, $mm2$
4: 4, $\overline{4}$
6: $\overline{3}$, 6, $\overline{6}$
6: 32, $3m$
8: mmm
8: $4/m$
Order 8: 422, $4mm$, $\overline{4}2m$
12: $6/m$
12: $\overline{3}m$, 622, $6mm$, $\overline{6}2m$
12: 23
16: $4/mmm$
24: $6/mmm$
24: $m\overline{3}$
24: 432, $\overline{4}3m$
48: $m\overline{3}m$.

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 $\overline{4}2m$ and $\overline{6}m2$ are described for two orientations with respect to the crystal axes, as $\overline{4}2m$ and $\overline{4}m2$ and as $\overline{6}m2$ and $\overline{6}2m$.
(*c*) The five trigonal point groups 3, $\overline{3}$, 32, $3m$ and $\overline{3}m$ 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 $\overline{3}m$ is given for two orientations, as 321 and 312, as $3m1$ and $31m$, and as $\overline{3}m1$ and $\overline{3}1m$; 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.

references