10.1. Crystallographic and noncrystallographic point groups

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10.1.1. Introduction and definitions

A *point group** 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.* Chapter 1.3); matrices for these symmetry operations are listed in Tables 11.2.2.1 and 11.2.2.2. 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 10.1.1.1 and 10.1.1.2. They are described in detail in Section 10.1.2. The two one-dimensional point groups are discussed in Section 2.2.17. The noncrystallographic point groups are treated in Section 10.1.4.

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);

(ii) in point space as site symmetries of points in lattices or in crystal structures and as symmetries of 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 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* is the set of all crystals having the same point-group symmetry. The word 'class', therefore, denotes a classificatory pigeon-hole 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 8.2.3 and 8.2.4.)

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 Part 3. For a given crystal, its Laue class is obtained if a symmetry centre is added to its point group, as shown in Table 10.2.1.1.

Table 10.1.1.1. *The ten two-dimensional crystallographic point groups, arranged according to crystal system*

Dashed lines separate 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	$2mm$	$4mm$	$3m$	$6mm$

In two dimensions, six 'centrosymmetric' crystallographic point groups and hence six two-dimensional Laue classes exist: 2; $2mm$; 4; $4mm$; 6; $6mm$. 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 *lattice point groups* (holohedral point groups, *holohedries*) are of special importance because they constitute the seven 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; $2mm$; $4mm$; $6mm$. Note that the hexagonal crystal family in two dimensions contains only one lattice type, with point symmetry $6mm$.

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:

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.

* 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 8.2.2. For a different use of the term 'point group' see Section 8.1.6.

references