Crystallographic point group

In crystallography, a **crystallographic point group** is a set of symmetry operations, corresponding to one of the point groups in three dimensions, such that each operation would leave the structure of a crystal unchanged i.e. the same kinds of atoms would be placed in similar positions as before the transformation. For example, in a primitive cubic crystal system, a rotation of the unit cell by 90 degree around an axis that is perpendicular to two parallel faces of the cube, intersecting at its center, is a symmetry operation that projects each atom to the location of one of its neighbor leaving the overall structure of the crystal unaffected.

In the classification of crystals, each point group defines a so-called **(geometric) crystal class**. There are infinitely many three-dimensional point groups. However, the crystallographic restriction on the general point groups results in there being only 32 crystallographic point groups. These 32 point groups are one-and-the-same as the 32 types of morphological (external) crystalline symmetries derived in 1830 by Johann Friedrich Christian Hessel from a consideration of observed crystal forms.

The point group of a crystal determines, among other things, the directional variation of physical properties that arise from its structure, including optical properties such as birefringency, or electro-optical features such as the Pockels effect. For a periodic crystal (as opposed to a quasicrystal), the group must maintain the three-dimensional translational symmetry that defines crystallinity.

Contents

Notation

The point groups are named according to their component symmetries. There are several standard notations used by crystallographers, mineralogists, and physicists.

For the correspondence of the two systems below, see **crystal system**.

Schoenflies notation

In Schoenflies notation, point groups are denoted by a letter symbol with a subscript. The symbols used in crystallography mean the following:

- C_n (for cyclic) indicates that the group has an n-fold rotation axis. C_{nh} is C_n with the addition of a mirror (reflection) plane perpendicular to the axis of rotation. C_{nv} is C_n with the addition of n mirror planes parallel to the axis of rotation.
- S_{2n} (for *Spiegel*, German for mirror) denotes a group with only a $2n$-fold rotation-reflection axis.
- D_n (for dihedral, or two-sided) indicates that the group has an n-fold rotation axis plus n twofold axes perpendicular to that axis. D_{nh} has, in addition, a mirror plane perpendicular to the n-fold axis. D_{nd} has, in addition to the elements of D_n, mirror planes parallel to the n-fold axis.
- The letter T (for tetrahedron) indicates that the group has the symmetry of a tetrahedron. T_d includes improper rotation operations, T excludes improper rotation operations, and T_h is T with the addition of an inversion.
- The letter O (for octahedron) indicates that the group has the symmetry of an octahedron (or cube), with (O_h) or without (O) improper operations (those that change handedness).

Due to the crystallographic restriction theorem, n = 1, 2, 3, 4, or 6 in 2- or 3-dimensional space.

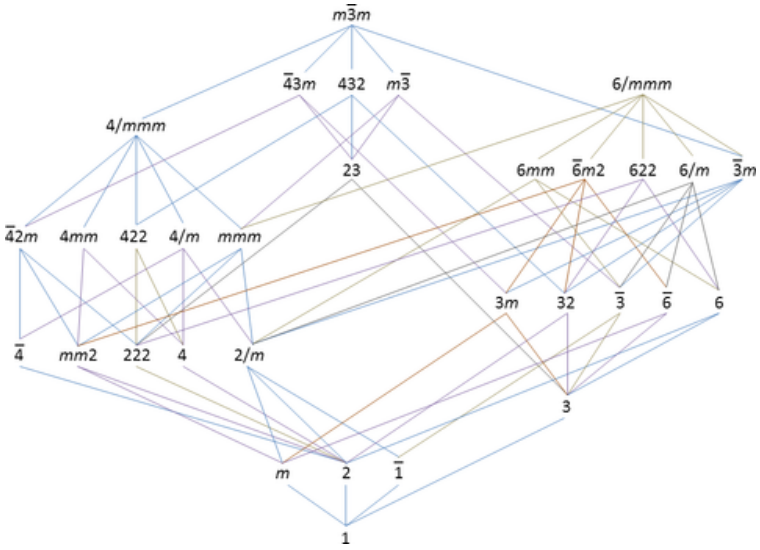
n	1	2	3	4	6
C_n	C_1	C_2	C_3	C_4	C_6
C_{nv}	$C_{1v}=C_{1h}$	C_{2v}	C_{3v}	C_{4v}	C_{6v}
C_{nh}	C_{1h}	C_{2h}	C_{3h}	C_{4h}	C_{6h}
D_n	$D_1=C_2$	D_2	D_3	D_4	D_6
D_{nh}	$D_{1h}=C_{2v}$	D_{2h}	D_{3h}	D_{4h}	D_{6h}
D_{nd}	$D_{1d}=C_{2h}$	D_{2d}	D_{3d}	D_{4d}	D_{6d}
S_{2n}	S_2	S_4	S_6	S_8	S_{12}

D_{4d} and D_{6d} are actually forbidden because they contain improper rotations with n=8 and 12 respectively. The 27 point groups in the table plus T, T_d, T_h, O and O_h constitute 32 crystallographic point groups.

Hermann–Mauguin notation

An abbreviated form of the Hermann–Mauguin notation commonly used for space groups also serves to describe crystallographic point groups. Group names are

Class	Group names						
Cubic	23	m$\bar{3}$		432	$\bar{4}$3m	m$\bar{3}$m	
Hexagonal	6	$\bar{6}$	$^6/_m$	622	6mm	$\bar{6}$m2	6/mmm
Trigonal	3	$\bar{3}$		32	3m	$\bar{3}$m	
Tetragonal	4	$\bar{4}$	$^4/_m$	422	4mm	$\bar{4}$2m	4/mmm
Orthorhombic				222		mm2	mmm
Monoclinic	2		$^2/_m$		m		
Triclinic	1	$\bar{1}$					



Subgroup relations of the 32 crystallographic point groups
(rows represent group orders from bottom to top as: 1,2,3,4,6,8,12,16,24, and 48.)

The correspondence between different notations

Crystal system	Hermann-Mauguin		Shubnikov[1]	Schoenflies	Orbifold	Coxeter	Order
	(full)	(short)					
Triclinic	1	1	$\mathbf{1}$	C_1	11	$[\,]^+$	1
	$\bar{1}$	$\bar{1}$	$\tilde{\mathbf{2}}$	$C_i = S_2$	×	$[2^+,2^+]$	2
Monoclinic	2	2	$\mathbf{2}$	C_2	22	$[2]^+$	2
	m	m	$\boldsymbol{m}$	$C_s = C_{1h}$	*	$[\,]$	2
	$\frac{2}{m}$	2/m	$\mathbf{2} : \boldsymbol{m}$	C_{2h}	2*	$[2,2^+]$	4
Orthorhombic	222	222	$\mathbf{2} : \mathbf{2}$	$D_2 = V$	222	$[2,2]^+$	4
	mm2	mm2	$\mathbf{2} \cdot \boldsymbol{m}$	C_{2v}	*22	$[2]$	4
	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	mmm	$\boldsymbol{m} \cdot \mathbf{2} : \boldsymbol{m}$	$D_{2h} = V_h$	*222	$[2,2]$	8
Tetragonal	4	4	$\mathbf{4}$	C_4	44	$[4]^+$	4
	$\bar{4}$	$\bar{4}$	$\tilde{\mathbf{4}}$	S_4	2×	$[2^+,4^+]$	4
	$\frac{4}{m}$	4/m	$\mathbf{4} : \boldsymbol{m}$	C_{4h}	4*	$[2,4^+]$	8
	422	422	$\mathbf{4} : \mathbf{2}$	D_4	422	$[4,2]^+$	8
	4mm	4mm	$\mathbf{4} \cdot \boldsymbol{m}$	C_{4v}	*44	$[4]$	8
	$\bar{4}$2m	$\bar{4}$2m	$\tilde{\mathbf{4}} \cdot \boldsymbol{m}$	$D_{2d} = V_d$	2*2	$[2^+,4]$	8
	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	4/mmm	$\boldsymbol{m} \cdot \mathbf{4} : \boldsymbol{m}$	D_{4h}	*422	$[4,2]$	16
Trigonal	3	3	$\mathbf{3}$	C_3	33	$[3]^+$	3
	$\bar{3}$	$\bar{3}$	$\tilde{\mathbf{6}}$	$C_{3i} = S_6$	3×	$[2^+,6^+]$	6
	32	32	$\mathbf{3} : \mathbf{2}$	D_3	322	$[3,2]^+$	6
	3m	3m	$\mathbf{3} \cdot \boldsymbol{m}$	C_{3v}	*33	$[3]$	6
	$\bar{3}\frac{2}{m}$	$\bar{3}$m	$\tilde{\mathbf{6}} \cdot \boldsymbol{m}$	D_{3d}	2*3	$[2^+,6]$	12
Hexagonal	6	6	$\mathbf{6}$	C_6	66	$[6]^+$	6
	$\bar{6}$	$\bar{6}$	$\mathbf{3} : \boldsymbol{m}$	C_{3h}	3*	$[2,3^+]$	6
	$\frac{6}{m}$	6/m	$\mathbf{6} : \boldsymbol{m}$	C_{6h}	6*	$[2,6^+]$	12
	622	622	$\mathbf{6} : \mathbf{2}$	D_6	622	$[6,2]^+$	12
	6mm	6mm	$\mathbf{6} \cdot \boldsymbol{m}$	C_{6v}	*66	$[6]$	12
	$\bar{6}$m2	$\bar{6}$m2	$\boldsymbol{m} \cdot \mathbf{3} : \boldsymbol{m}$	D_{3h}	*322	$[3,2]$	12
	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	6/mmm	$\boldsymbol{m} \cdot \mathbf{6} : \boldsymbol{m}$	D_{6h}	*622	$[6,2]$	24
Cubic	23	23	$\mathbf{3/2}$	T	332	$[3,3]^+$	12
	$\frac{2}{m}\bar{3}$	m$\bar{3}$	$\tilde{\mathbf{6}}/\mathbf{2}$	T_h	3*2	$[3^+,4]$	24
	432	432	$\mathbf{3/4}$	O	432	$[4,3]^+$	24
	$\bar{4}$3m	$\bar{4}$3m	$\mathbf{3}/\tilde{\mathbf{4}}$	T_d	*332	$[3,3]$	24
	$\frac{4}{m}\bar{3}\frac{2}{m}$	m$\bar{3}$m	$\tilde{\mathbf{6}}/\mathbf{4}$	O_h	*432	$[4,3]$	48

Deriving the crystallographic point group (crystal class) from the space group

1. Leave out the Bravais type
2. Convert all symmetry elements with translational components into their respective symmetry elements without translation symmetry (Glide planes are converted into simple mirror planes; Screw axes are converted into simple axes of rotation)
3. Axes of rotation, rotoinversion axes and mirror planes remain unchanged.

See also

- Molecular symmetry
- Point group
- Space group
- Point groups in three dimensions

- Crystal system

References

1. "Archived copy" (https://archive.is/20130704042455/http://it.iucr.org/Ab/ch12o1v0001/sec12o1o3/). Archived from the original (http://it.iucr.org/Ab/ch12o1v0001/sec12o1o3/) on 2013-07-04. Retrieved 2011-11-25.

External links

- Point-group symbols in International Tables for Crystallography (2006). Vol. A, ch. 12.1, pp. 818-820 (https://archive.is/20130704033345/http://it.iucr.org/Ab/ch12o1v0001/)
- Names and symbols of the 32 crystal classes in International Tables for Crystallography (2006). Vol. A, ch. 10.1, p. 794 (https://archive.is/20130704032551/http://it.iucr.org/Ab/ch10o1v0001/table10o1o2o4/)
- Pictorial overview of the 32 groups (https://web.archive.org/web/20120204104121/http://newton.ex.ac.uk/research/qsystems/people/goss/symmetry/Solids.html)