

and two sets of vertical mirror planes, one set through the axes C_4 and denoted by $2\sigma_v$ and the other set through the bisectors of the $2\sigma_v$ planes and denoted by the dihedral vertical mirror planes $2\sigma_d$. Table 3.11 is useful in relating the two kinds of notations for rotations and improper rotations.

3.11 Symmetry Relations and Point Group Classifications

In this section we summarize some useful relations between symmetry operations and give the classification of point groups. Some useful relations on the commutativity of symmetry operations are:

- (a) Inversion commutes with all point symmetry operations.
- (b) All rotations about the same axis commute.
- (c) All rotations about an arbitrary rotation axis commute with reflections across a plane perpendicular to this rotation axis.
- (d) Two twofold rotations about perpendicular axes commute.
- (e) Two reflections in perpendicular planes will commute.
- (f) Any two of the symmetry elements σ_h , S_n , C_n ($n = \text{even}$) implies the third.

If we have a major symmetry axis C_n ($n \geq 2$) and there are either twofold axes C_2 or vertical mirror planes σ_v , then there will generally be more than one C_2 or σ_v symmetry operations. In some cases these symmetry operations are in the same class and in the other cases they are not, and this distinction can be made by use of conjugation (see Sect. 1.6).

The classification of the 32 crystallographic point symmetry groups shown in Table 3.12 is often useful in making practical applications of character tables in textbooks and journal articles to specific materials.

In Table 3.12 the first symbol in the Hermann–Mauguin notation denotes the principal axis or plane. The second symbol denotes an axis (or plane) perpendicular to this axis, except for the cubic groups, where the second symbol refers to a $\langle 111 \rangle$ axis. The third symbol denotes an axis or plane that is \perp to the first axis and at an angle of π/n with respect to the second axis.

In addition to the 32 crystallographic point groups that are involved with the formation of three-dimensional crystals, there are nine symmetry groups that form clusters and molecules which show icosahedral symmetry or are related to the icosahedral group I_h . We are interested in these species because they can become part of crystallographic structures. Examples of such clusters and molecules are fullerenes. The fullerene C_{60} has full icosahedral symmetry I_h (Table A.28), while C_{70} has D_{5h} symmetry (Table A.26) and C_{80} has D_{5d} symmetry (Table A.25). The nine point groups related to icosahedral symmetry that are used in solid state physics, as noted earlier, are also listed in Table 3.12 later that double line.

Table 3.12. The extended 32 crystallographic point groups and their symbols^(a)

system	Schoenflies	Hermann–Mauguin symbol ^(b)		examples
	symbol	full	abbreviated	
triclinic	C_1 $C_i, (S_2)$	1 $\bar{1}$	1 $\bar{1}$	Al_2SiO_5
monoclinic	$C_{1h}, (S_1)$ C_2 C_{2h}	m 2 $2/m$	m 2 $2/m$	KNO_2
orthorhombic	C_{2v} $D_2, (V)$ $D_{2h}, (V_h)$	$2mm$ 222 $2/m\ 2/m\ 2/m$	mm 222 mmm	I, Ga
tetragonal	C_4 S_4 C_{4h} $D_{2d}, (V_d)$ C_{4v} D_4 D_{4h}	4 $\bar{4}$ $4/m$ $\bar{4}2m$ $4mm$ 422 $4/m\ 2/m\ 2/m$	4 $\bar{4}$ $4/m$ $\bar{4}2m$ $4mm$ 42 $4/mmm$	CaWO_4 $\text{TiO}_2, \text{In}, \beta\text{-Sn}$
rhombohedral	C_3 $C_{3i}, (S_6)$ C_{3v} D_3 D_{3d}	3 $\bar{3}$ $3m$ 32 $\bar{3}2/m$	3 $\bar{3}$ $3m$ 32 $\bar{3}m$	AsI_3 FeTiO_3 Se Bi, As, Sb, Al_2O_3
hexagonal	$C_{3h}, (S_3)$ C_6 C_{6h} D_{3h} C_{6v} D_6 D_{6h}	$\bar{6}$ 6 $6/m$ $\bar{6}2m$ $6mm$ 622 $6/m\ 2/m\ 2/m$	$\bar{6}$ 6 $6/m$ $\bar{6}2m$ $6mm$ 62 $6/mmm$	 ZnO, NiAs CeF_3 Mg, Zn, graphite

Footnote (a): The usual 32 crystallographic point groups are here extended by including 9 groups with 5 fold symmetry and are identified here as icosahedral point groups.

Footnote (b): In the Hermann–Mauguin notation, the symmetry axes parallel to and the symmetry planes perpendicular to each of the “principal” directions in the crystal are named in order. When there is both an axis parallel to and a plane normal to a given direction, these are indicated as a fraction; thus $6/m$ means a sixfold rotation axis standing perpendicular to a plane of symmetry, while $\bar{4}$ denotes a fourfold rotary inversion axis. In some classifications, the rhombohedral (trigonal) groups are listed with the hexagonal groups. Also shown are the corresponding entries for the icosahedral groups (see text).

Table 3.12. (continued)

the extended 32 crystallographic point groups and their symmetries				
system	Schoenflies	Hermann–Mauguin symbol		examples
	symbol	full	abbreviated	
cubic	T	23	23	NaClO ₃
	T_h	$2/m\bar{3}$	$m\bar{3}$	FeS ₂
	T_d	$\bar{4}3m$	$\bar{4}3m$	ZnS
	O	432	43	β -Mn
	O_h	$4/m\bar{3}2/m$	$m\bar{3}m$	NaCl, diamond, Cu
icosahedral	C_5	5	5	
	$C_{5i}, (S_{10})$	$\bar{10}$	$\bar{10}$	
	C_{5v}	$5m$	$5m$	
	C_{5h}, S_5	$\bar{5}$	$\bar{5}$	
	D_5	52	52	
	D_{5d}	$\bar{5}2/m$	$\bar{5}/m$	C_{80}
	D_{5h}	$\bar{10}2m$	$\bar{10}2m$	C_{70}
	I	532	532	
	I_h			C_{60}

It is also convenient to picture many of the point group symmetries with stereograms (see Fig. 3.2). The stereogram is a mapping of a general point on a sphere onto a plane going through the center of the sphere. If the point on the sphere is above the plane it is indicated as $a +$, and if below as $a \circ$. In general, the polar axis of the stereogram coincides with the principal axis of symmetry. The first five columns of Fig. 3.2 pertain to the crystallographic point group symmetries and the sixth column is for fivefold symmetry.

The five first stereograms on the first row pertaining to groups with a single axis of rotation show the effect of two-, three-, four-, and sixfold rotation axes on a point $+$. These groups are cyclic groups with only n -fold axes. Note the symmetry of the central point for each group. On the second row we have added vertical mirror planes which are indicated by the solid lines. Since the “vertical” and “horizontal” planes are not distinguishable for C_1 , the addition of a mirror plane to C_1 is given in the third row, showing the groups which result from the first row upon addition of horizontal planes. The symbols \oplus indicate the coincidence of the projection of points above and below the plane, characteristic of horizontal mirror planes.

If instead of proper rotations as in the first row, we can also have improper rotations, then the groups on row 4 are generated. Since S_1 is identical with C_{1h} , it is not shown separately; this also applies to $S_3 = C_{3h}$ and to $S_5 = C_{5h}$ (neither of which are shown). It is of interest to note that S_2 and S_6 have inversion symmetry but S_4 does not.

The addition of twofold axes \perp to the principal symmetry axis for the groups in the first row yields the stereograms of the fifth row where the twofold

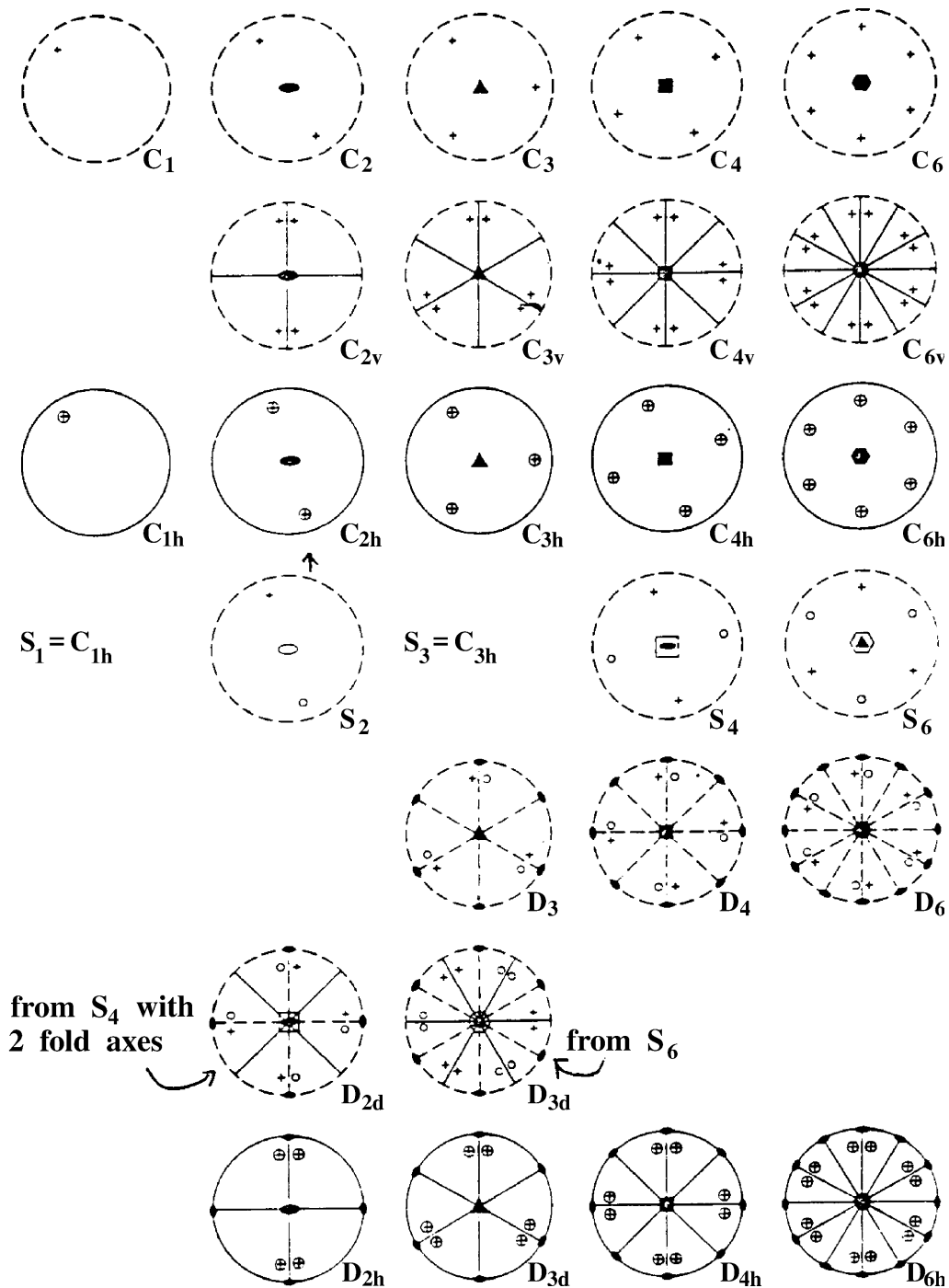


Fig. 3.2. The first five columns show stereographic projections of simple crystallographic point groups

axes appear as dashed lines. Here we see that the higher the symmetry of the principal symmetry axis, the greater the number of twofold axes D_5 (not shown) that would have 5 axes separated by 72° .

The addition of twofold axes to the groups on the fourth row yields the stereograms of the sixth row, where D_{2d} comes from S_4 , while D_{3d} comes from S_6 . Also group D_{5d} (not shown) comes from S_{10} . The addition of twofold axes