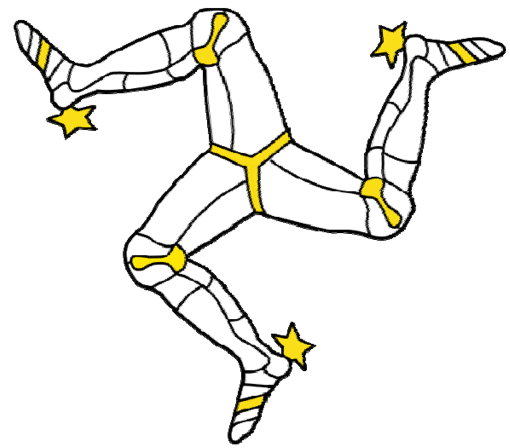
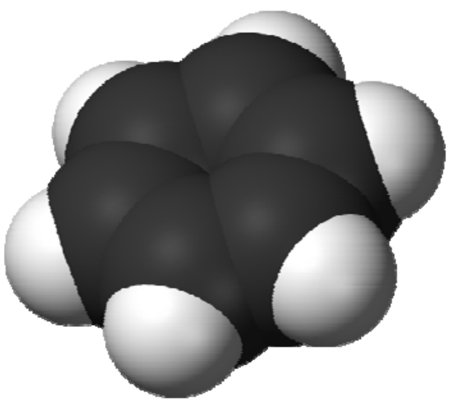
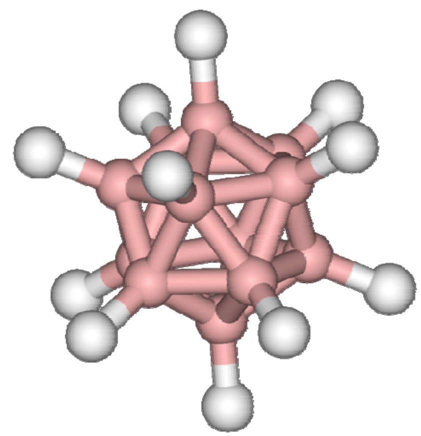
Lecture 12 February 11, 2019

- ***Symmetry in Nature and in Molecules***
- ***Symmetry Operations***
- ***Symmetry Elements***
- ***Point Groups and Assignments***

Symmetry







Intuitively, we know symmetry when we see it.

But how do we put in quantitative terms that allows us to compare, assign, classify?

Symmetry in Nature and in Molecules

The symmetry of a molecule is determined by the existence of **symmetry operations** performed with respect to **symmetry elements**. A ***symmetry element*** is a line, a plane or a point within or through an object, intersecting at a specific point (hence ***point groups***) about which a rotation or reflection leaves the object in an orientation indistinguishable from the original. A ***plane*** of symmetry is designated by the symbol **σ** (or sometimes s), and the reflection operation is the coincidence of atoms on one side of the plane with corresponding atoms on the other side, as though reflected in a mirror. A ***center or point of symmetry is labeled i,*** and the inversion operation demonstrates coincidence of each atom with an identical one on a line passing through and an equal distance from the inversion point. Finally, a ***rotational axis is designated C_n***, where the degrees of rotation that restore the object is 360/n (C_2= 180º rotation, C_3= 120º rotation, C_4= 90º rotation, C_5= 72º rotation). C_1 is called the identity operation **E** because it returns the original orientation.

An object having no symmetry elements other than E is called **asymmetric**. Such an object is necessarily chiral. Since a plane or point of symmetry involves a reflection operation, the presence of such an element makes an object **achiral**. One or more rotational axes of symmetry may exist in both chiral, **dissymmetric**, and achiral objects.

Symmetry Operations and Symmetry Elements

Definitions:

- A **symmetry operation** is an operation on a body such that, after the operation has been carried out, the result is indistinguishable from the original body (every point of the body is coincident with an equivalent point or the same point of the body in its original orientation).
- A **symmetry element** is a geometrical entity such as a line, a plane, or a point, with respect to which one or more symmetry operations may be carried out

Symmetry Operation	Symmetry Element	Notation
Identity	-	E
Reflection in a plane	Plane of symmetry	σ_v, σ_d, σ_h
Proper rotation	Rotation axis (line)	C_n ; where = 360/angle
Rotation followed by reflection in the plane perpendicular to the rotation axis	Improper rotation axis (line)	S_n
Inversion	Center of inversion	I

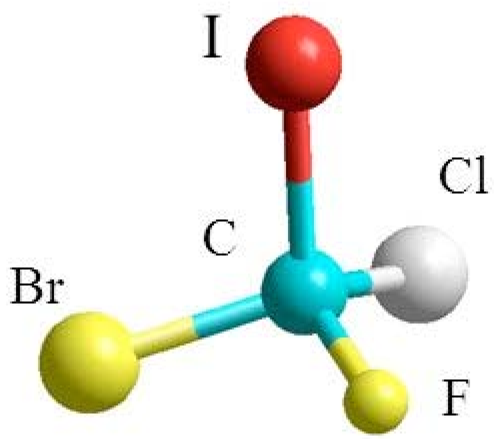
Let’s look for these in molecules

What is a point group? A collection of symmetry elements for a specific symmetry, intersecting at a specific point for molecules, and displayed in a character table.

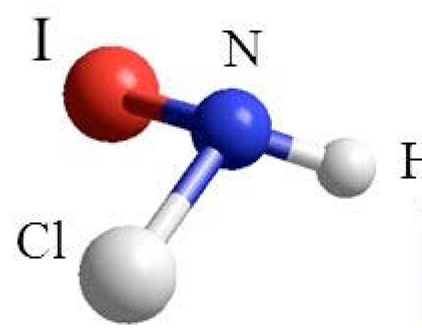
The C_1 point group:

Molecules that have no symmetry elements at all except the trivial one where they are rotated through 360º and remain unchanged, belong to the C_1 point group. In other words, they have an axis of 360º/360º = 1-fold, so have a C_1 axis. Examples are:

C_1



Bromo-chloro-fluoro-iodo-methane



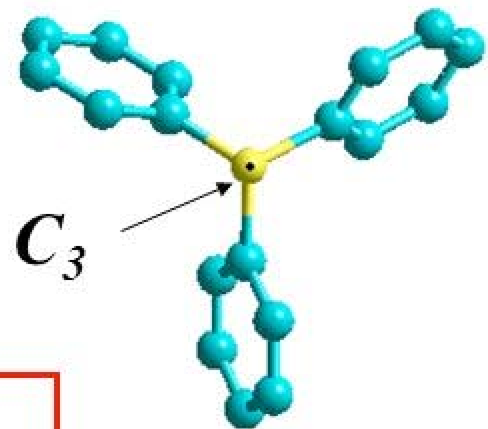
C_1

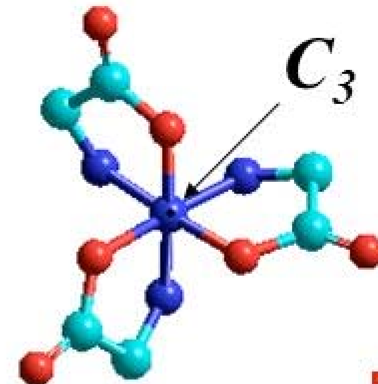
chloro-iodo-amine

The C_n point groups:

These have a C_n axis as their only symmetry element. They generally resemble propellers which have the front and back different. Important examples are (hydrogens omitted for clarity):

triphenyl phosphine viewed down C_3 axis



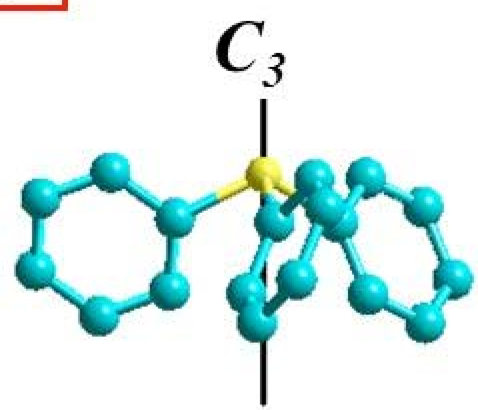


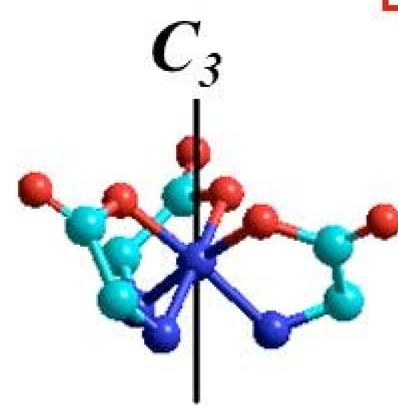
Cobalt(III) tris-glycinate viewed down C_3 axis

C_3

C_3

triphenyl phosphine viewed from the side





Cobalt(III) tris-glycinate viewed from the side

Notes

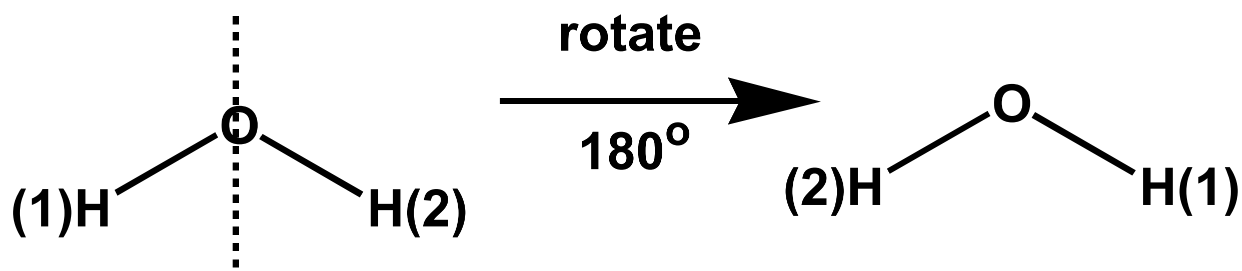
(i) symmetry operations more fundamental, but elements often easier to spot.

(ii) some symmetry elements give rise to more than one operation - especially rotation - as above.

ROTATIONS - AXES OF SYMMETRY

Some examples for different types of molecule: e.g.

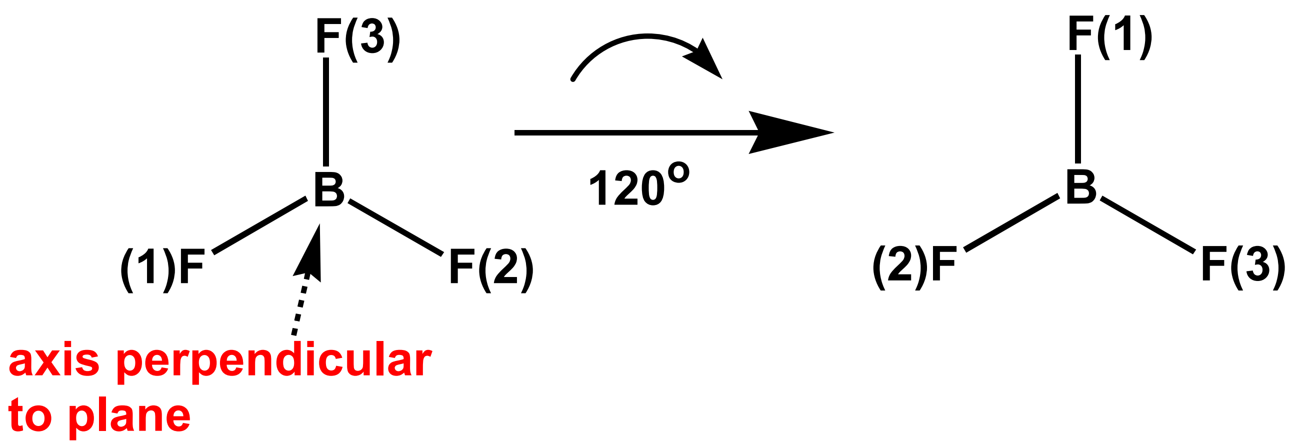
H_2O



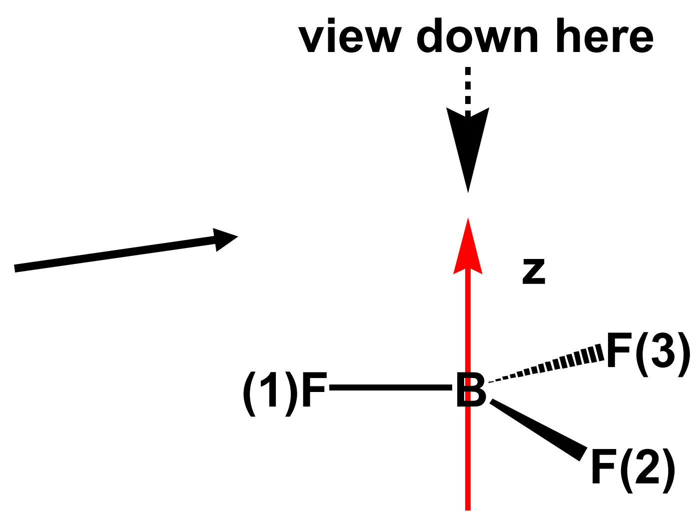
Line in molecular plane, bisecting HOH angle is a rotation axis, giving indistinguishable configuration on rotation by 180°.

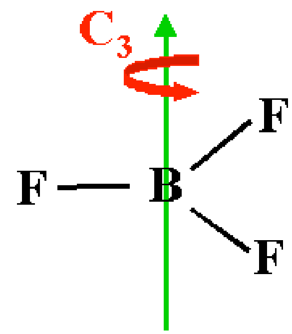
BF_3

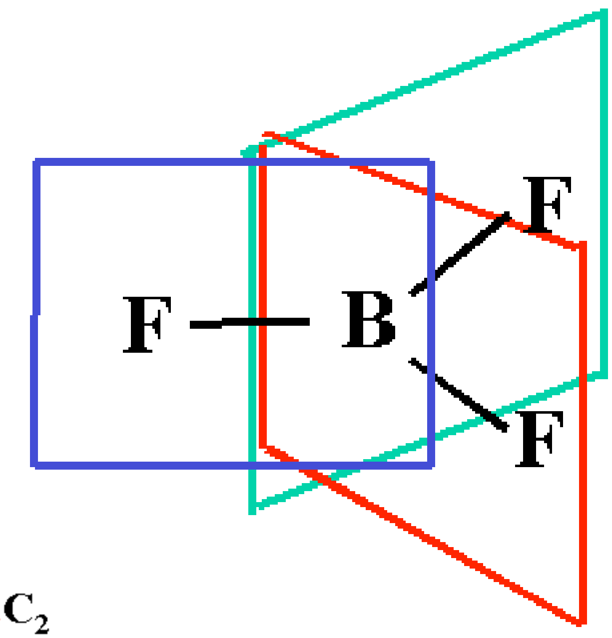
By VSEPR - trigonal, planar, all bonds equal, all angles 120°. Take as axis a line perpendicular to molecular plane, passing through B atom.

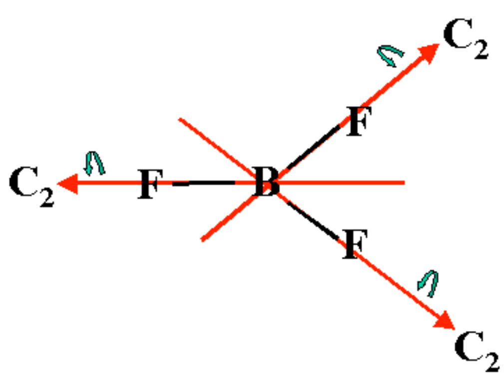


N.B. all rotations CLOCKWISE when viewed along -z direction.




C3
F
B
F
F


F
B
F
F

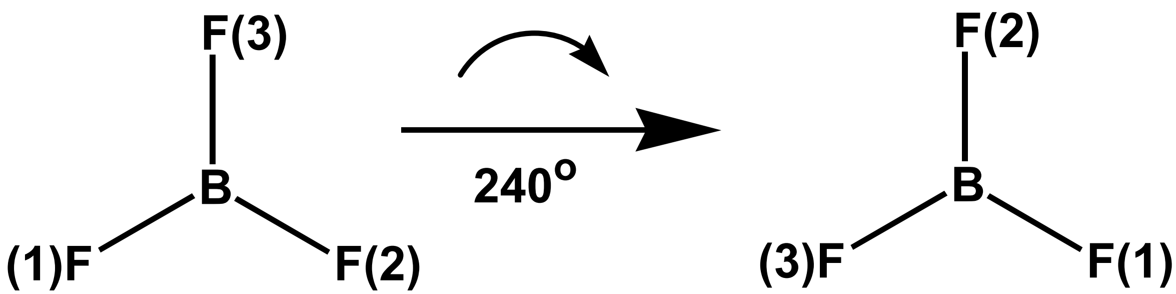

C2
F
B
F
F
C2
C2

Symbol for axes of symmetry

C_n

where rotation about axis gives indistinguishable configuration every $(360/n)^o$ (i.e. an n-fold axis)

Thus H_2O has a C_2 (two-fold) axis, BF_3 a C_3 (three-fold) axis. One axis can give rise to >1 rotation, e.g. for BF_3, what if we rotate by 240^o?



Must differentiate between two operations.

Rotation by 120^o described as C_3^1,

rotation by 240^o as C_3^2.

In general C_n axis (minimum angle of rotation $(360/n)^o$) gives operations C_n^m, where both m and n are integers.

When m = n we have a special case, which introduces a new type of symmetry operation.....

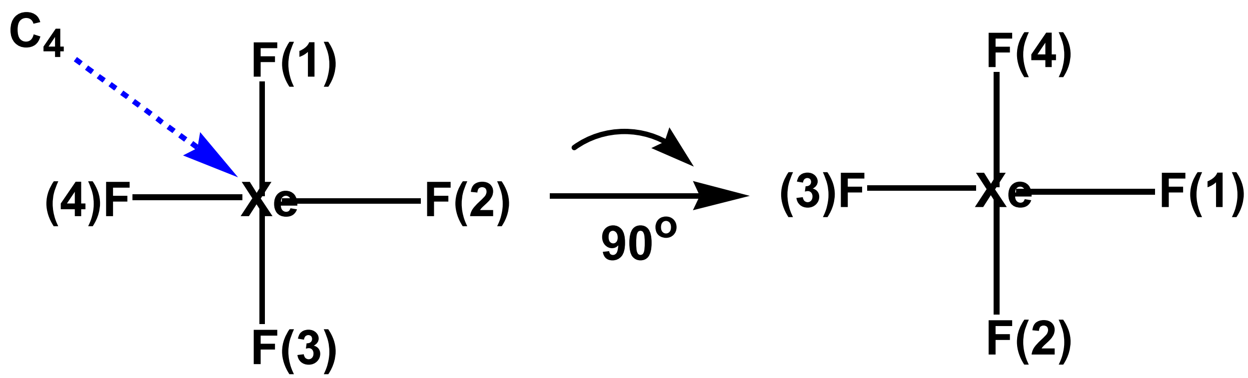
IDENTITY OPERATION

For H_2O, C_2^2 and for BF_3 C_3^3 both bring the molecule to an IDENTICAL arrangement to initial one.

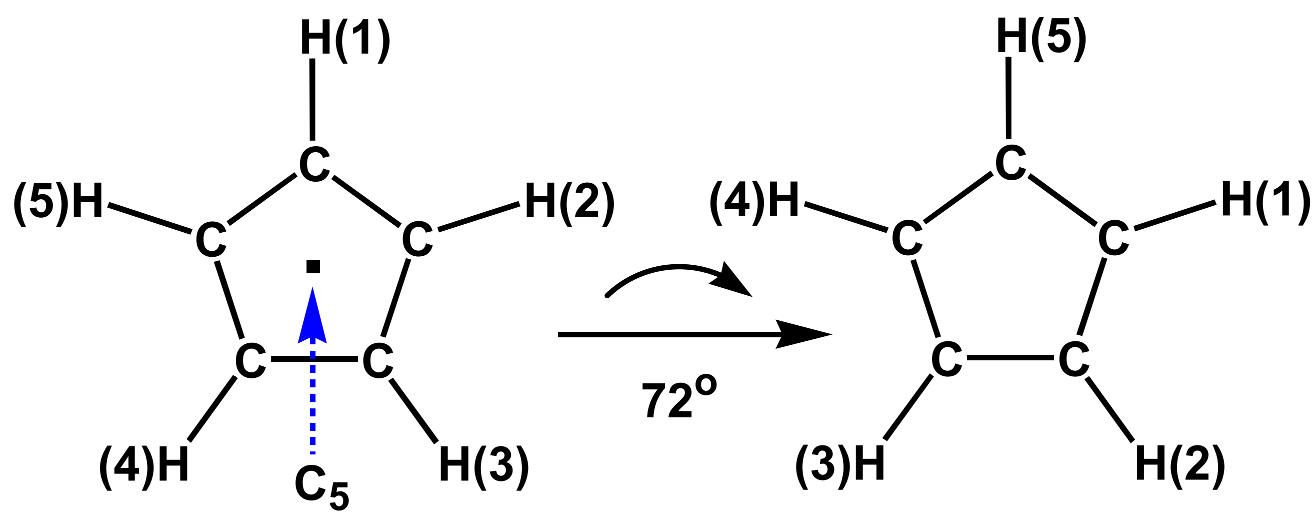
Rotation by 360^o is exactly equivalent to rotation by 0^o, i.e. the operation of doing NOTHING to the molecule.

MORE ROTATION AXES

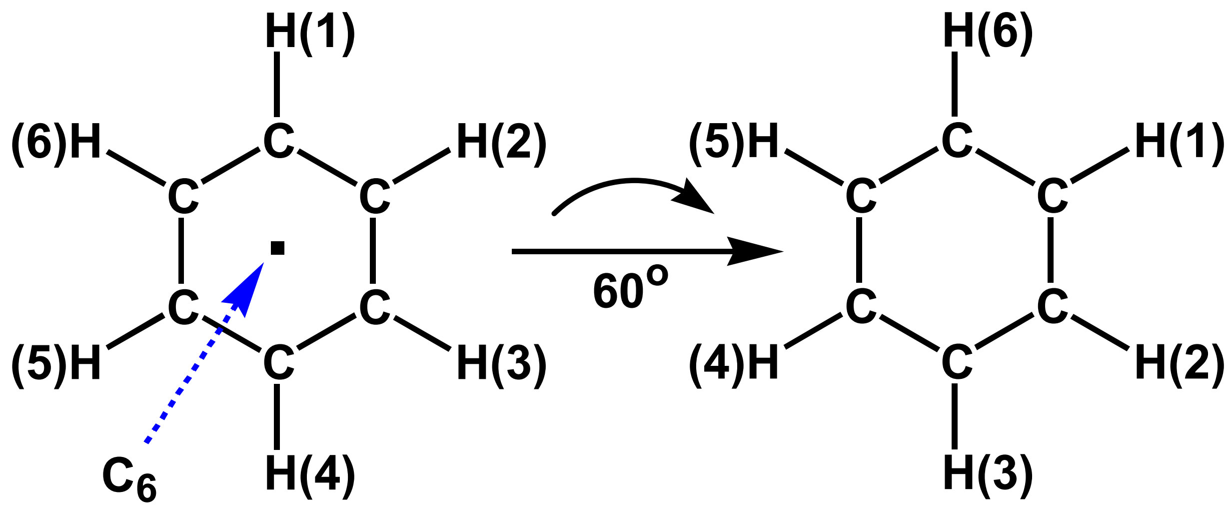
xenon tetrafluoride, XeF_4



cyclopentadienide ion, $C_5H_5^-$

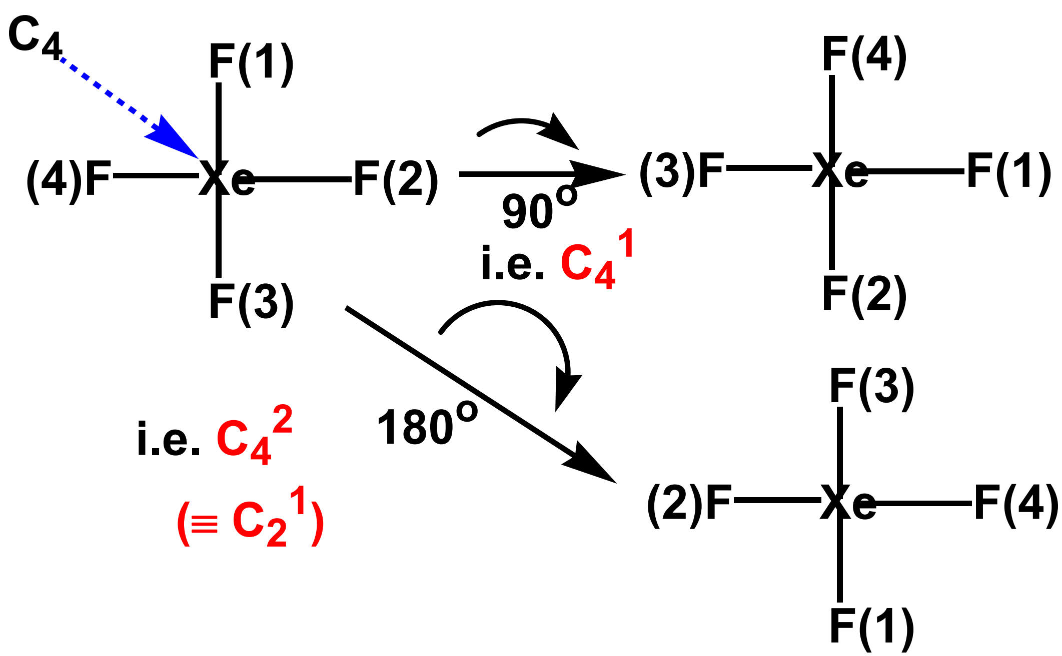


benzene, C_6H_6



Examples also known of C_7 and C_8 axes.

If a C_{2n} axis (i.e. even order) present, then C_n must also be present:



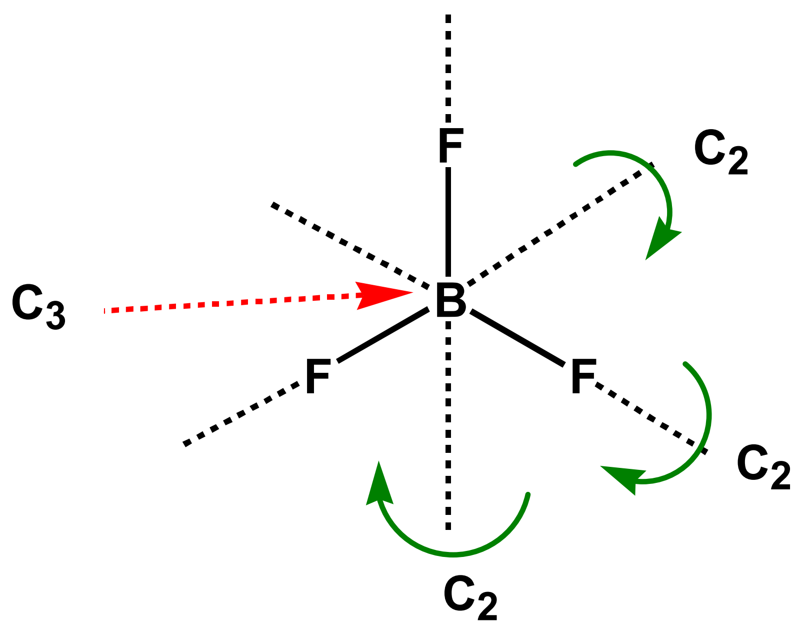
Therefore there must be a C_2 axis coincident with C_4, and the operations generated by C_4 can be written:

C_4^1, C_4^2 (C_2^1), C_4^3, C_4^4 (E)

Similarly, a C_6 axis is accompanied by C_3 and C_2, and the operations generated by C_6 are:

C_6^1, C_6^2 (C_3^1), C_6^3 (C_2^1), C_6^4 (C_3^2), C_6^5, C_6^6 (E)

Molecules can possess several distinct axes, **e.g. BF_3:**



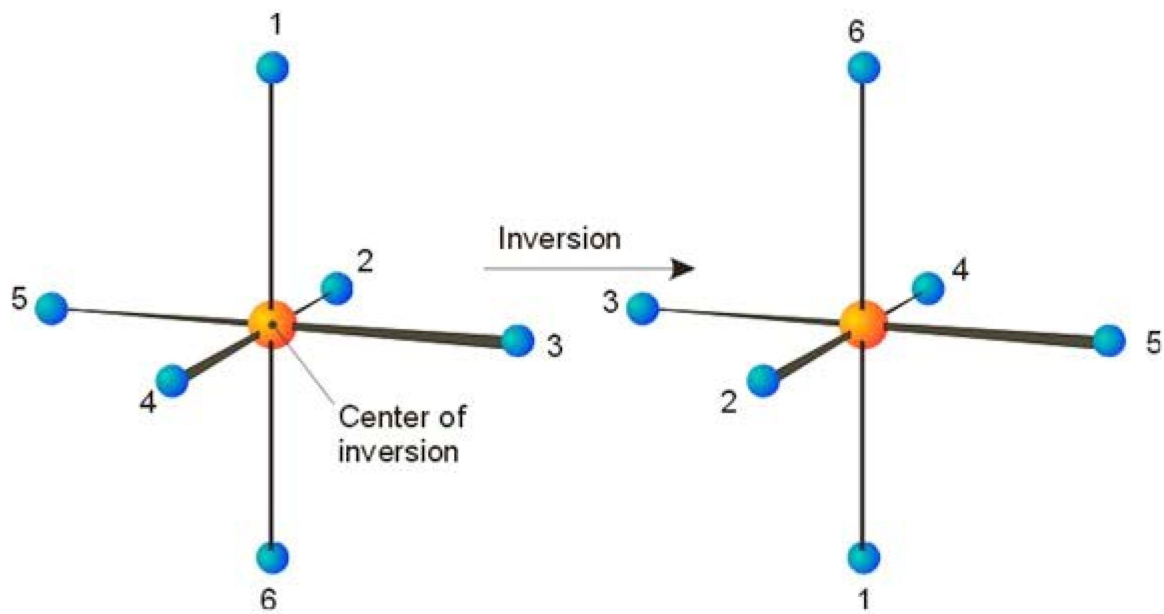
Three C_2 axes, one along each B-F bond, perpendicular to C_3

n C_2 perpendicular to C_n puts molecule in D point group

Inversion (i)

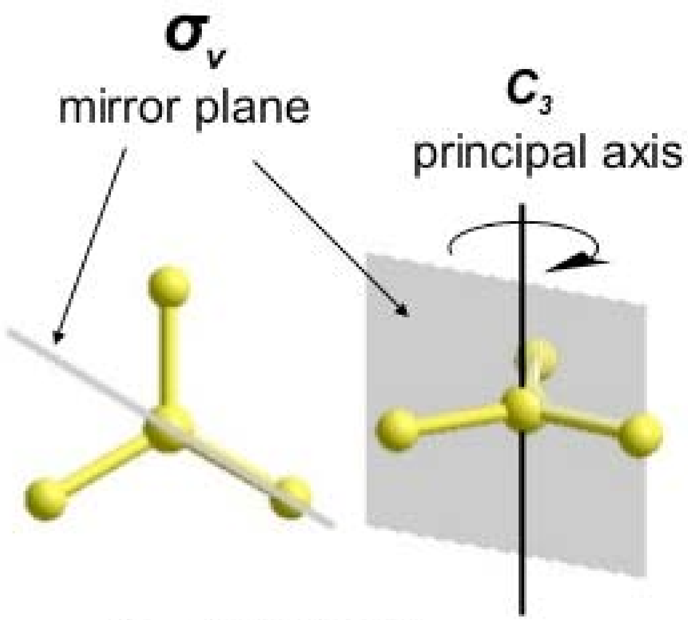
Each atom in the molecule is moved along a straight line through the inversion center to a point an equal distance from the inversion center.

X,Y,Z → -X, -Y, -Z

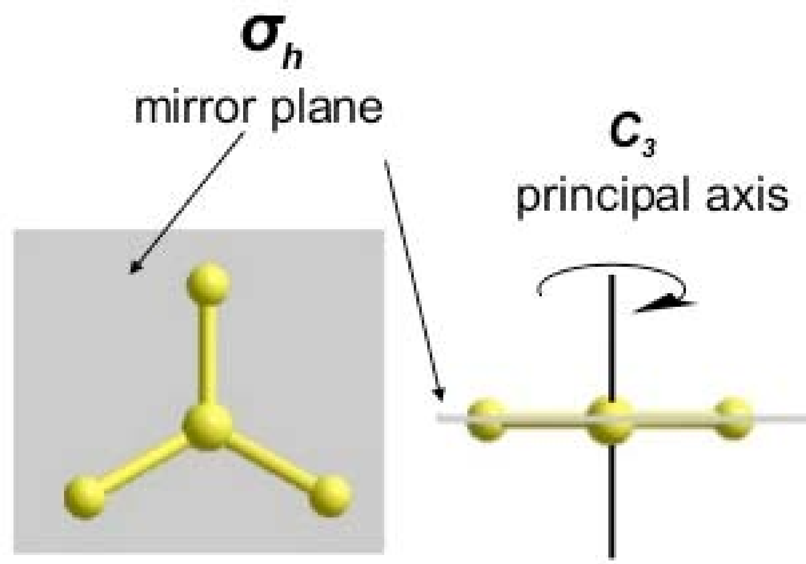


Mirror planes (σ) of BF_3:

Mirror planes can contain the principal axis (σ_v) or be at right angles to it (σ_h). BF_3 has one σ_h and three σ_v planes: (*v* = vertical, *h* = horizontal)

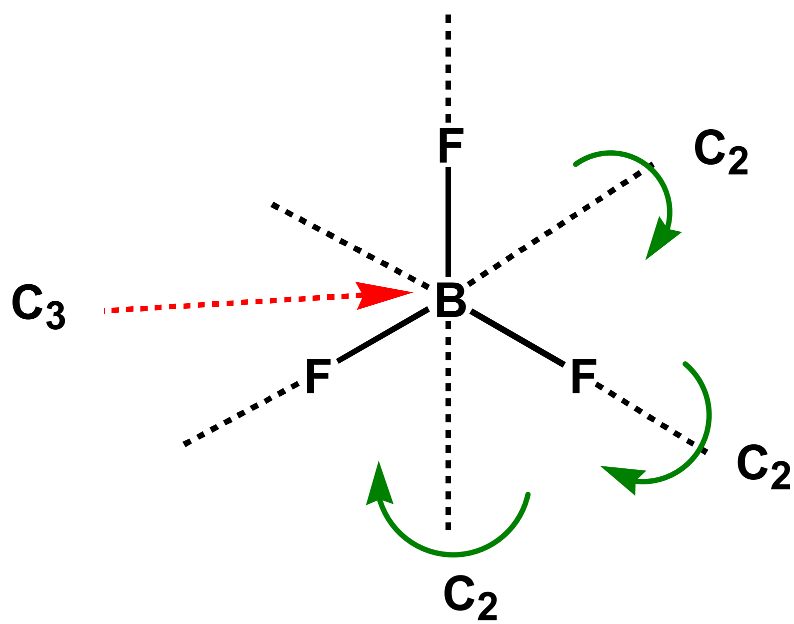


σ_v mirror plane
contains the C_3 axis



σ_h mirror plane
is at right angles to the C_3 axis

Molecules can possess several distinct axes, **e.g.** **BF_3:**



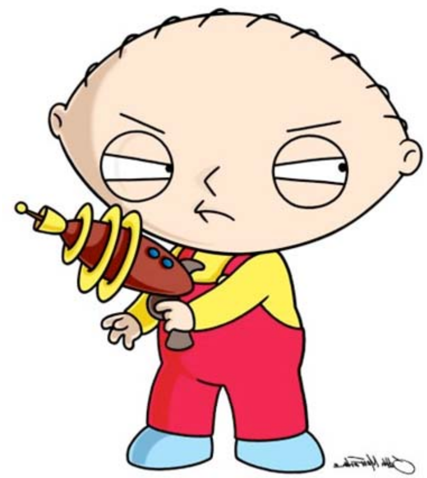
Three C_2 axes, one along each B-F bond, perpendicular to C_3

n C_2 perpendicular to C_n puts molecule in D point group

Symmetry elements/operations can be manipulated by
Group Theory, Representations and Character Tables

So, What IS a group?

And, What is a Character???



A GROUP is a collection of entities or elements which satisfy the following four conditions:

1) The product of any two elements (including the square of each element) must be an element of the group. For symmetry operations, the multiplication rule is to successively perform operations.

2) One element in the group must commute with all others and leave them unchanged. Therefore the "E",

$$EX = XE = X$$

3) The associative law of multiplication must hold

$$A(BC) = (AB)C$$

4) Every element must have a reciprocal which is also an element of the group. i.e.,

$$X(X^{-1}) = (X^{-1})X = E$$

Note: An element may be its own reciprocal.

Groups may be composed of anything: symmetry operations, nuclear particles, etc. Simplest is +1, -1.

All the groups which follow the same multiplication table are called representations of the same group. → ***Character Tables***

W. H. FREEMAN

Table 6.4 The C_{2v} character table

C_{2v}	E	C_2	σ_v	σ_v'	$h = 4$	
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	–1	–1	R_z	
B_1	1	–1	1	–1	x, R_y	xy
B_2	1	–1	–1	1	y, R_x	zx, yz

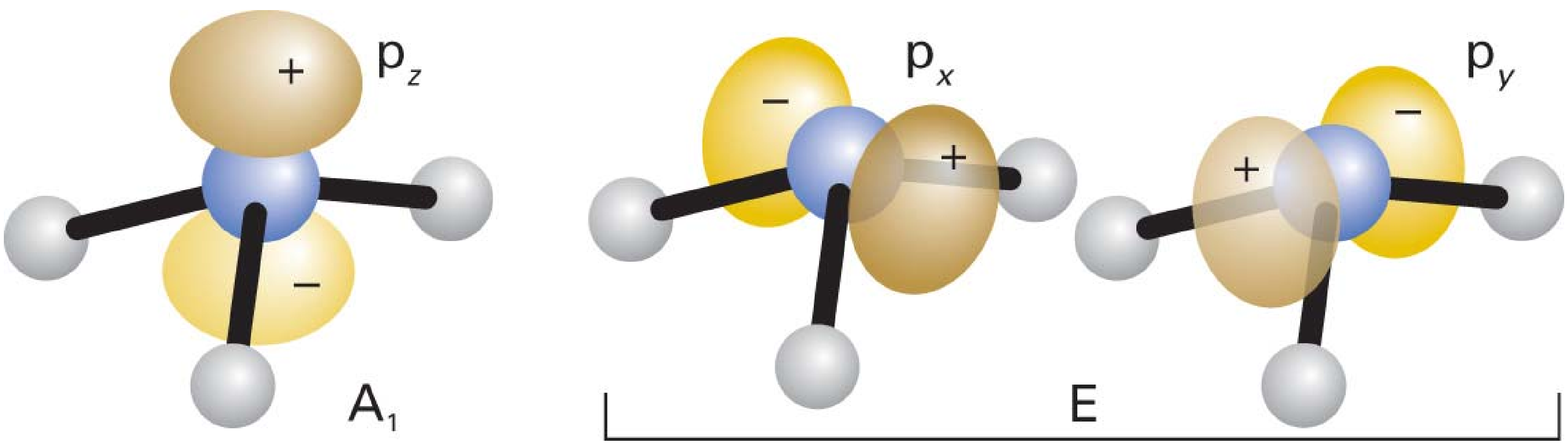
Table 6.3 The components of a character table

Name of point group*	Symmetry operations R arranged by class (E, C_n, etc.)	Functions	Further functions	Order of group, h
Symmetry species (Γ)	Characters (χ)	Translations and components of dipole moments (x, y, z), of relevance to IR activity; rotations	Quadratic functions such as z^2, xy, etc., of relevance to Raman activity	

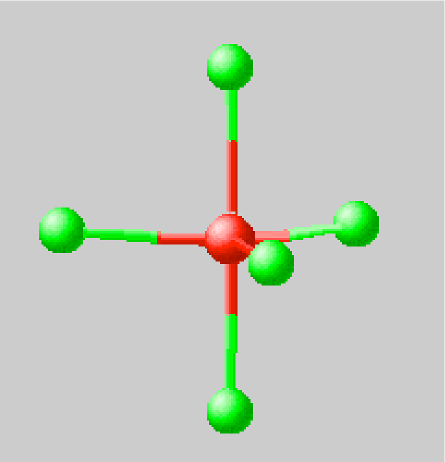
* Schoenflies symbol.

Character table for point group C_{3v}

C_{3v}	E	$2C_3$ (z)	$3\sigma_v$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	z	x^2+y^2, z^2	z^3, $x(x^2-3y^2)$, $z(x^2+y^2)$
A_2	+1	+1	-1	R_z	-	$y(3x^2-y^2)$
E	+2	-1	0	(x, y) (R_x, R_y)	(x^2-y^2, xy) (xz, yz)	(xz^2, yz^2) [xyz, $z(x^2-y^2)$] [$x(x^2+y^2)$, $y(x^2+y^2)$]



D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)



Character table for D_{4h} point group

	E	$2C_4$ (z)	C_2	$2C'_2$	$2C''_2$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	linears, rotations	quadratic
A_{1g}	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		x^2-y^2
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0	(x, y)	

Consequences of Symmetry

- Only the molecules which belong to the $\mathbf{C_n}$, $\mathbf{C_{nv}}$, or $\mathbf{C_s}$ **point** group can have a permanent dipole moment.
- A molecule may be chiral only if it does not have an axis of improper rotation $\mathbf{S_n}$.
- IR Allowed transitions may be predicted by symmetry operations
- Orbital overlap may be predicted and described by symmetry

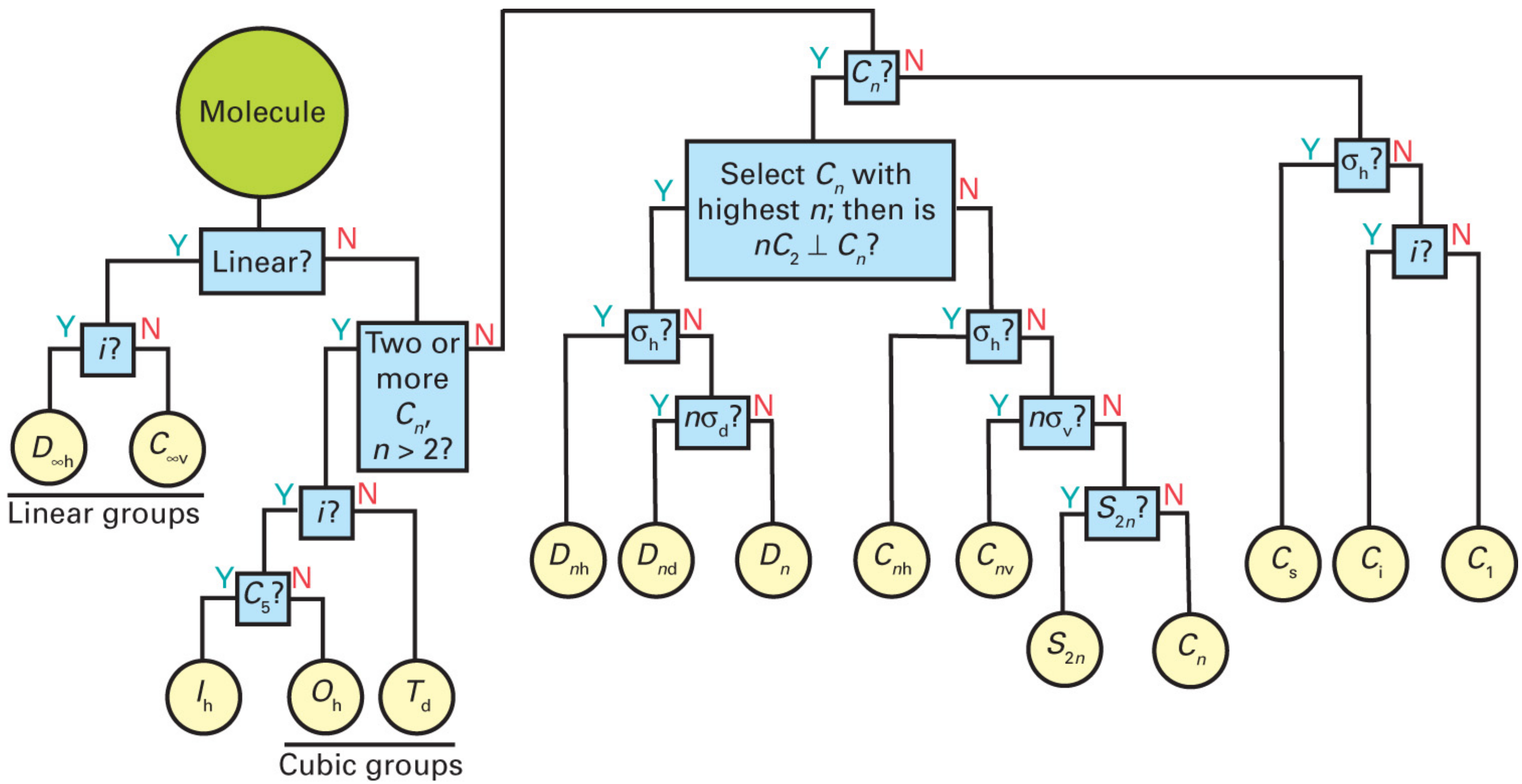
Point Group Assignments and Character Tables

POINT GROUPS

A collection of symmetry operations all of which pass through a single point

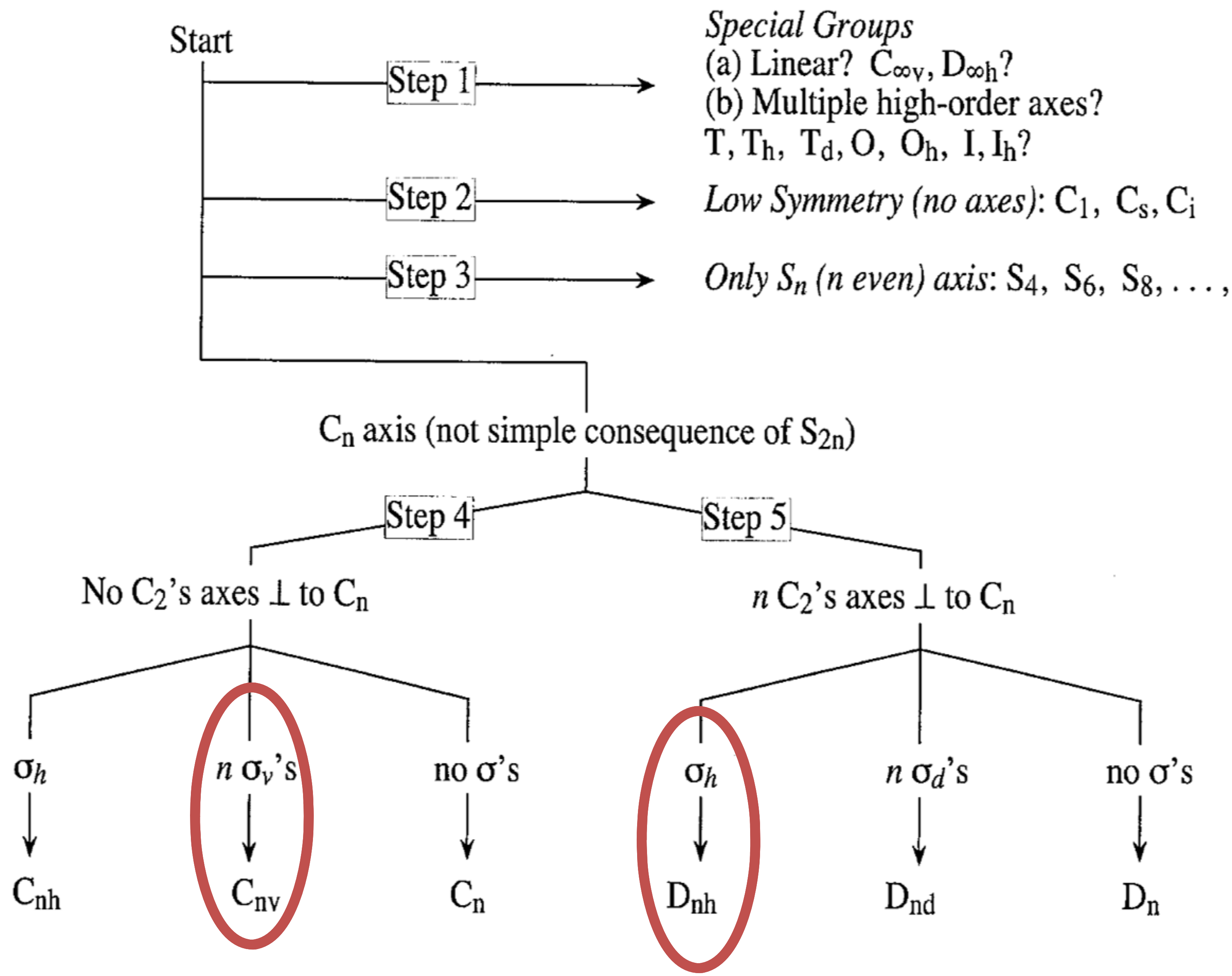
A point group for a molecule is a quantitative measure of the symmetry of that molecule

Assignment of Symmetry Elements to Point Group: At first Looks Daunting.



Daunting? However almost all we will be concerned with belong to just a few symmetry point groups

A Simpler Approach



POINT GROUPS

A collection of symmetry operations all of which pass through a single point

A point group for a molecule is a quantitative measure of the symmetry of that molecule

ASSIGNMENT OF MOLECULES TO POINT GROUPS

STEP 1 : LOOK FOR AN AXIS OF SYMMETRY

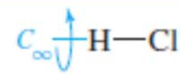
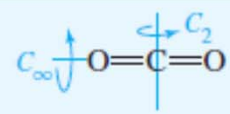
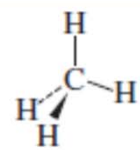
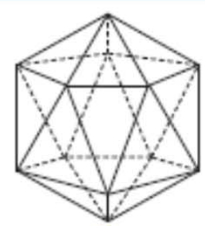
If one is found - go to STEP 2

If not: look for

(a) plane of symmetry - if one is found, molecule belongs to point group C_s

Point Group Assignments: Weller, Armstrong Ch. 3

TABLE 4.3 Groups of High Symmetry

Group	Description	Examples
$C_{\infty v}$	These molecules are linear, with an infinite number of rotations and an infinite number of reflection planes containing the rotation axis. They do not have a center of inversion.	
$D_{\infty h}$	These molecules are linear, with an infinite number of rotations and an infinite number of reflection planes containing the rotation axis. They also have perpendicular C_2 axes, a perpendicular reflection plane, and an inversion center.	
T_d	Most (but not all) molecules in this point group have the familiar tetrahedral geometry. They have four C_3 axes, three C_2 axes, three S_4 axes, and six σ_d planes. They have no C_4 axes.	
O_h	These molecules include those of octahedral structure, although some other geometrical forms, such as the cube, share the same set of symmetry operations. Among their 48 symmetry operations are four C_3 rotations, three C_4 rotations, and an inversion.	
I_h	Icosahedral structures are best recognized by their six C_5 axes, as well as many other symmetry operations—120 in all.	 $B_{12}H_{12}^{2-}$ with BH at each vertex of an icosahedron

In addition, there are four other groups, T, T_h, O, and I, which are rarely seen in nature. These groups are discussed at the end of this section.

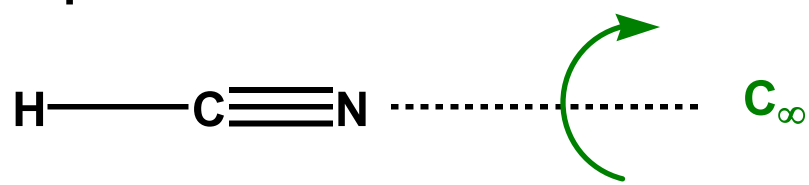
LINEAR MOLECULES

Do in fact fit into scheme - but they have an infinite number of symmetry operations.

Molecular axis is C_∞ - rotation by any arbitrary angle $(360/\infty)^o$, so infinite number of rotations. Also any plane containing axis is symmetry plane, so infinite number of planes of symmetry.

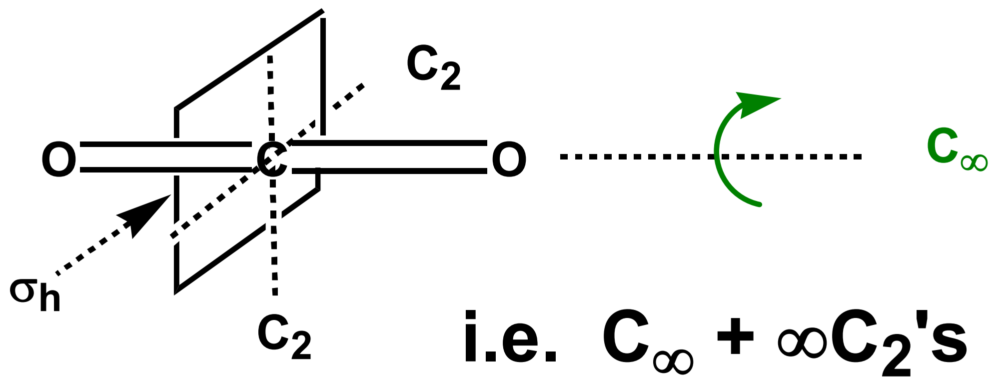
Divide linear molecules into two groups:

(i) No centre of symmetry, e.g.:



No C_2's perp. to main axis, but ∞ σ_v's containing main axis: point group $C_{\infty v}$

(ii) Centre of symmetry, e.g.:



i.e. $C_\infty + \infty C_2\text{'s} + \sigma_h$

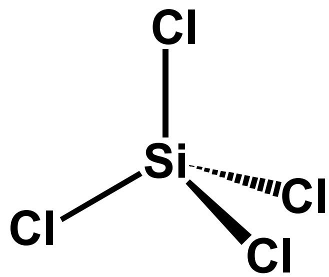
Point group $D_{\infty h}$

Highly symmetrical molecules

A few geometries have several, equivalent, highest order axes. Two geometries most important:

Regular tetrahedron

e.g.

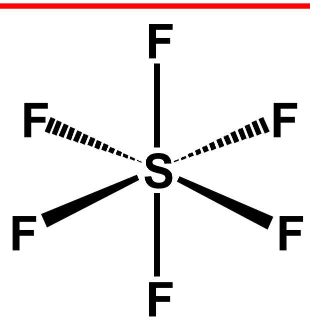


4 C_3 axes (one along each bond)
3 C_2 axes (bisecting pairs of bonds)
3 S_4 axes (coincident with C_2's)
6 σ_d's (each containing Si and 2 Cl's)

Point group: T_d

Regular octahedron

e.g.



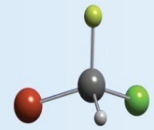
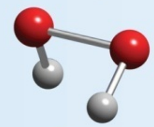
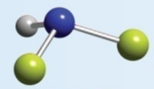
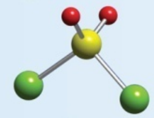
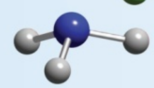
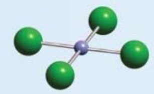
3C_4's (along F-S-F axes)
also 4 C_3's. 6 C_2's, several planes, S_4, S_6 axes, and a centre of symmetry (at S atom)

Point group O_h

These molecules can be identified without going through the usual steps.

Note: many of the more symmetrical molecules possess many more symmetry operations than are needed to assign the point group.

Table 6.2 The composition of some common groups

Point group	Symmetry elements	Shape	Examples
C_1	E		SiHClBrF
C_2	E, C_2		H_2O_2
C_s	E, σ		NHF_2
C_{2v}	$E, C_2, \sigma_v, \sigma_v'$		SO_2Cl_2, H_2O
C_{3v}	$E, 2C_3, 3\sigma_v$		NH_3, PCl_3, $POCl_3$
$C_{\infty v}$	$E, C_2, 2C_\varphi, \infty\sigma_v$		OCS, CO, HCl
D_{2h}	$E, 3C_2, i, 3\sigma$		N_2O_4, B_2H_6
D_{3h}	$E, 2C_3, 3C_2, \sigma_h, 2S_3, 3\sigma_v$		BF_3, PCl_5
D_{4h}	$E, 2C_4, C_2, 2C_2', 2C_2'', i, 2S_4, \sigma_h, 2\sigma_v, 2\sigma_d$		XeF_4, *trans*-$[MA_4B_2]$
$D_{\infty h}$	$E, \infty C_2', 2C_\varphi, i, \infty\sigma_v, 2S_\varphi$		CO_2, H_2, C_2H_2
T_d	$E, 8C_3, 3C_2, 6S_4, 6\sigma_d$		CH_4, $SiCl_4$
O_h	$E, 8C_3, 6C_2, 6C_4, 3C_2, i, 6S_4, 8S_6, 3\sigma_h, 6\sigma_d$		SF_6

4. The C_{nv} Groups

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	R_z	
E	2	−1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	−1	−1	R_z	
B_1	1	−1	1	1	−1		$x^2 - y^2$
B_2	1	−1	1	−1	1		xy
E	2	0	−2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	−1	R_z	
E_1	2	2 cos 72°	2 cos 144°	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	2 cos 144°	2 cos 72°	0		$(x^2 - y^2, xy)$

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	1	−1		
B_2	1	−1	1	−1	−1	1		
E_1	2	1	−1	−2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	−1	−1	2	0	0		$(x^2 - y^2, xy)$

4. The C_{nv} Groups

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	R_z	
E	2	−1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	−1	−1	R_z	
B_1	1	−1	1	1	−1		$x^2 - y^2$
B_2	1	−1	1	−1	1		xy
E	2	0	−2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	−1	R_z	
E_1	2	2 cos 72°	2 cos 144°	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	2 cos 144°	2 cos 72°	0		$(x^2 - y^2, xy)$

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	1	−1		
B_2	1	−1	1	−1	−1	1		
E_1	2	1	−1	−2	0	0	$(x, y)(R_x, R_y)$	(xz, yz)
E_2	2	−1	−1	2	0	0		$(x^2 - y^2, xy)$

6. The D_{nh} Groups

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	xz
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1	R_z	
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1		$x^2 - y^2$
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1		xy
E_g	2	0	−2	0	0	2	0	−2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	z	
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1		
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1		
E_u	2	0	−2	0	0	−2	0	2	0	0	(x, y)	

5. The D_{nh} Groups

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	xz
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1	R_z	
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1		$x^2 - y^2$
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1		xy
E_g	2	0	−2	0	0	2	0	−2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	z	
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1		
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1		
E_u	2	0	−2	0	0	−2	0	2	0	0	(x, y)	

9. The Cubic Groups (Continued).

T_h	E	$4C_3$	$4C_3^2$	$3C_2$	i	$4S_6$	$4S_6^5$	$3\sigma_h$		$\varepsilon = \exp(2\pi i/3)$
A_g	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A_u	1	1	1	1	-1	-1	-1	-1		
E_g	1	ε	ε^*	1	1	ε	ε^*	1		$(2z^2-x^2-y^2,$
	1	ε^*	ε	1	1	ε^*	ε	1		$x^2-y^2)$
E_u	1	ε	ε^*	1	-1	$-\varepsilon$	$-\varepsilon^*$	-1		
	1	ε^*	ε	1	-1	$-\varepsilon^*$	$-\varepsilon$	-1		
T_g	3	0	0	-1	3	0	0	-1	(R_x, R_y, R_z)	(xz, yz, xy)
T_u	3	0	0	-1	-3	0	0	1	(x, y, z)	

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2-x^2-y^2,$ $x^2-y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)

O	E	$6C_4$	$3C_2(=C_4^2)$	$8C_3$	$6C_2$		
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	-1	1	1	-1		
E	2	0	2	-1	0		$(2z^2-x^2-y^2,$ $x^2-y^2)$
T_1	3	1	-1	0	-1	(R_x, R_y, R_z); (x, y, z)	
T_2	3	-1	-1	0	1		(xy, xz, yz)

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
E_g	2	-1	0	0	2	2	0	-1	2	0		$(2z^2-x^2-y^2,$ $x^2-y^2)$.
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1		(xz, yz, xy)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1		
E_u	2	-1	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		

Table 6.4 The C_{2v} character table

C_{2v}	E	C_2	σ_v	σ_v'	$h = 4$	
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	–1	–1	R_z	
B_1	1	–1	1	–1	x, R_y	xy
B_2	1	–1	–1	1	y, R_x	zx, yz

Table 6.5 The C_{3v} character table

C_{3v}	E	$2C_3$	$3\sigma_v$	$h = 6$	
A_1	1	1	1	z	z^2
A_2	1	1	−1	R_z	
E	2	−1	0	(x, y) (R_x, R_y)	(zx, yz) $(x^2 - y^2, xy)$

Character table for $C_{\infty v}$ point group

	E	**$2C_\infty$**	**...**	**∞ &sigma$_v$**	**linear, rotations**	**quadratic**
$A_1=\Sigma^+$	1	1	...	1	z	x^2+y^2, z^2
$A_2=\Sigma^-$	1	1	...	-1	R_z	
$E_1=\Pi$	2	2cos(Φ)	...	0	(x, y) (R_x, R_y)	(xz, yz)
$E_2=\Delta$	2	2cos(2ϕ)	...	0		(x^2-y^2, xy)
$E_3=\Phi$	2	2cos(3ϕ)	...	0		
...	...	...	...	...		

Character table for $D_{\infty h}$ point group

	E	$2C_\infty$	...	$\infty\sigma_v$	i	$2S_\infty$	...	$\infty C'_2$	linear functions, rotations	quadratic
$A_{1g}=\Sigma^+_g$	1	1	...	1	1	1	...	1		x^2+y^2, z^2
$A_{2g}=\Sigma^-_g$	1	1	...	-1	1	1	...	-1	R_z	
$E_{1g}=\Pi_g$	2	2cos(ϕ)	...	0	2	-2cos(ϕ)	...	0	(R_x, R_y)	(xz, yz)
$E_{2g}=\Delta_g$	2	2cos(2ϕ)	...	0	2	2cos(2ϕ)	...	0		(x^2-y^2, xy)
$E_{3g}=\Phi_g$	2	2cos(3ϕ)	...	0	2	-2cos(3ϕ)	...	0		
...	...	...	...	...	...	...	...	...		
$A_{1u}=\Sigma^+_u$	1	1	...	1	-1	-1	...	-1	z	
$A_{2u}=\Sigma^-_u$	1	1	...	-1	-1	-1	...	1		
$E_{1u}=\Pi_u$	2	2cos(ϕ)	...	0	-2	2cos(ϕ)	...	0	(x, y)	
$E_{2u}=\Delta_u$	2	2cos(2ϕ)	...	0	-2	-2cos(2ϕ)	...	0		
$E_{3u}=\Phi_u$	2	2cos(3ϕ)	...	0	-2	2cos(3ϕ)	...	0		
...	...	...	...	...	...	...	...	...		