Symmetry

CHEM 2430

n-fold rotation axis $\rightarrow$ rotation by 360°/n (C_n)

C_n symmetry element

$\hat{C}_n$ symmetry operation

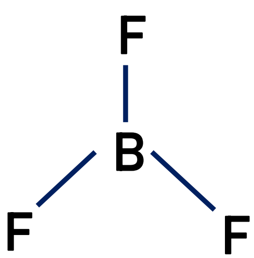
Reflection plane (σ)

Inversion(i)

Not present in BF_3

Present in H_2, C_2H_4, etc.

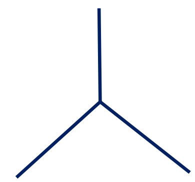
n-fold improper rotation (n–fold rotation + reflection) (S_n)



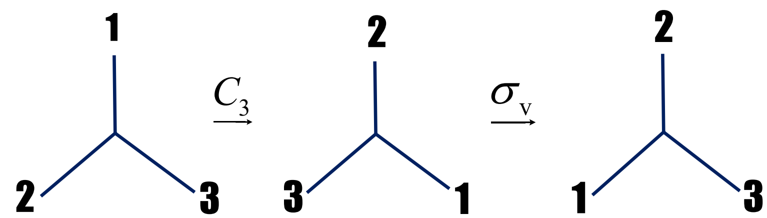
Has three σ_v one σ_h reflection planes

There are also C_3, C_3^{-1} (or C_3^2) and three C_2 operations.

All groups have the identity (E) operation.



C_3 axis is also S_3 axis



CH_4 has a three S_4 axis that are not a C_4 axis

A product of two symmetry operations = a symmetry operation in the group

If a molecule belongs to a particular group all symmetry operations in the group commute with it.

C_1 only $\hat{E}$

C_s only $\hat{E}, \hat{\sigma}_h$

C_i only $\hat{E}, \hat{i}$

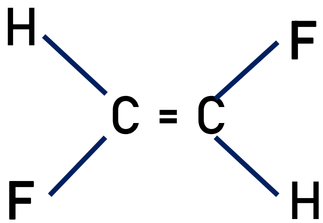
C_n only $\hat{E}, \hat{C}_n, \hat{C}_n^{\ 2}, \ldots \hat{C}_n^{\ n-1}$

C_2 has $\hat{E}, \hat{C}_2$

C_3 has $\hat{E}, \hat{C}_3, \hat{C}_3^{\ 2}$ etc.

C_{nh} has a symmetry plane $(\sigma_h) \perp$ to C_n axis

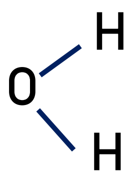
C_{2h}



also has inversion

C_{nv} C_n plus n vertical symmetry planes passing through C_n

C_{2v}



$E, \sigma_{\mathrm{v}}, \sigma_h, C_2$

Examples of point groups

C_s	E	σ_h		
A'	1	1	x, y	x^2, y^2, z^2, xy
A''	1	-1	z	yz, xz

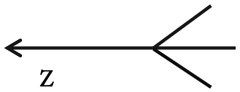
C_{2v}	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1		xy
B_1	1	-1	1	-1	x	xz
B_2	1	-1	-1	1	y	yz

Product of two representations is a representation

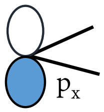
$$B_1 \times B_2 = (1, 1, -1, -1) = A_2$$

Different representations are orthogonal

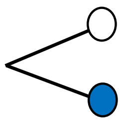
$$B_1 \cdot B_2 = 1 + 1 - 1 - 1 = 0$$



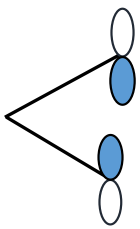
water molecule in the *yz* plane



belongs to B_1



belongs to B_2



belongs to A_2

p orbitals here are perpendicular to the plane

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

C_3 and C_3^2 are the same type of operation and are grouped together. Ditto for the three σ_v operations

Show E $\perp$ to A_1 : $(2)(1)+2(-1)(1)+3(0)(1)=2-2=0$

What representation is $E^2 = \begin{pmatrix} 4 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 1 & -1 \end{pmatrix}$

$$E^2 \Rightarrow E + A_1 + A_2$$

For a heteronuclear diatomic, the point group is $C_{\infty v}$

This group lacks the I and C_2 operations.

$D_{\infty h}$	E	$2C_\infty$	…	$\infty\sigma_v$	$2S_\infty$	i	…	∞C_2		
Σ_g^+	1	1	…	1	1	1	…	1		x^2+y^2, z^2
Σ_g^-	1	1	…	-1	1	1	…	-1		
Π_g	2	$2\cos\phi$	…	0	2	$-2\cos\phi$	…	0		(xz, yz)
⋮										
Σ_u^+	1	1	…	1	-1	-1	…	-1		
Σ_u^-	1	1	…	-1	-1	-1	…	1	z	
Π_u	2	$2\cos\phi$	…	0	-2	$2\cos\phi$	…	0	(x, y)	

$\left(x^2-y^2, xy\right)$ belongs to Δ_g