(13) **Today**

4.1 Symmetry elements and Operations

4.2 Point Groups

4.3 Properties and Representations of Groups

Next Class (14)

4.3 Properties and Representations of Groups

(15) **Second Class from Today**

4.3 Properties and Representations of Groups

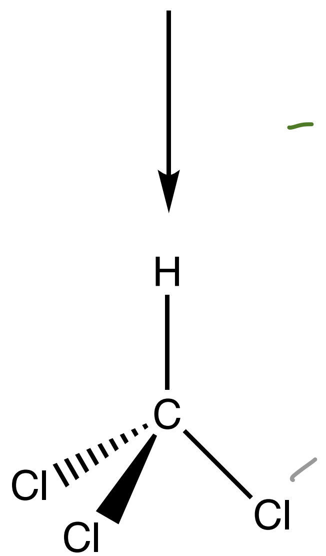
4.4 Uses of Character Tables

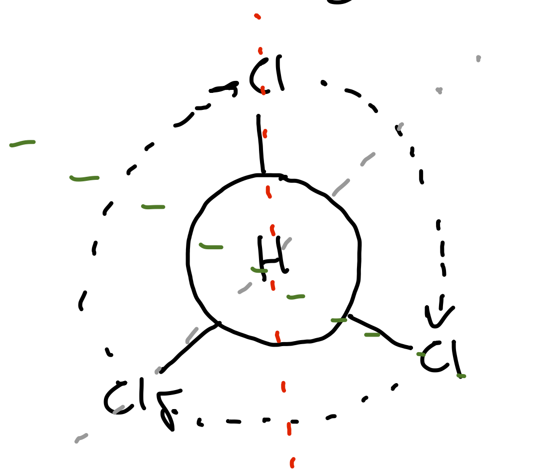
Third Class from Today (16)

4.4 Uses of Character Tables

C_3
120° or $\frac{1}{3}$ of a circle

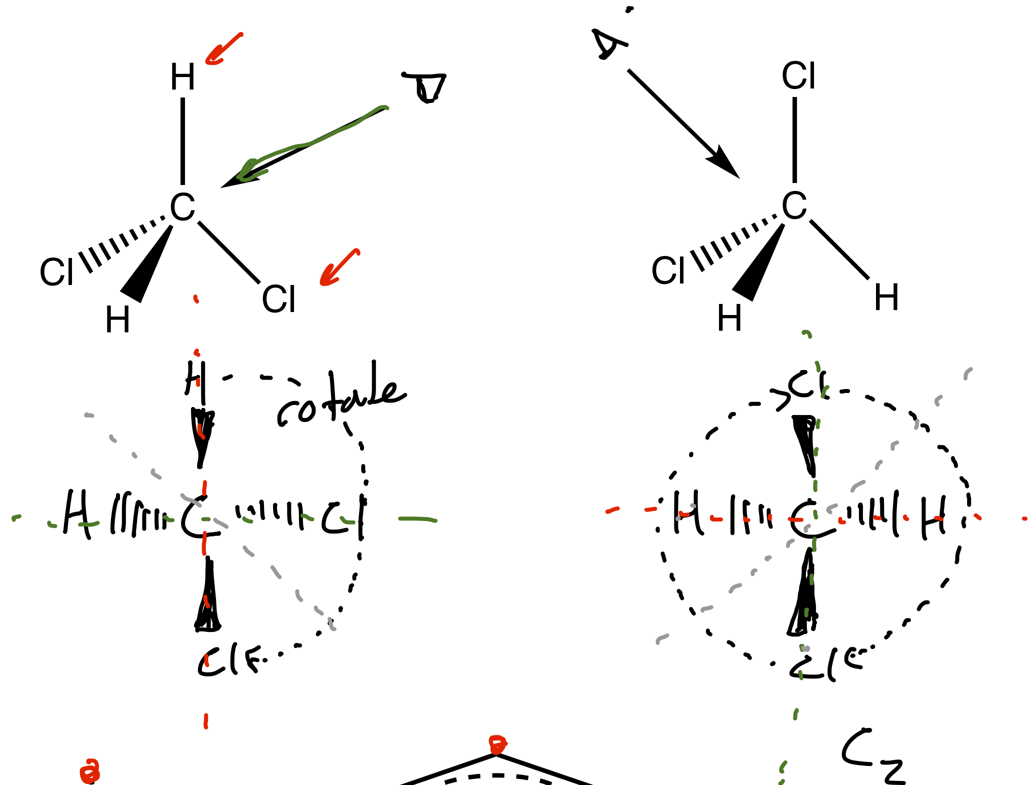
Look along bonds





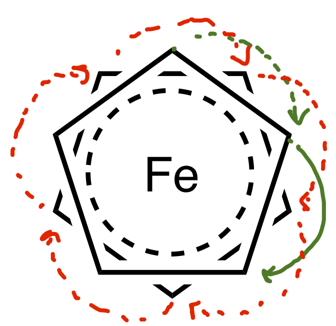
mirror plane...
cut in half same? yes

Look along lines that bisect bond angles

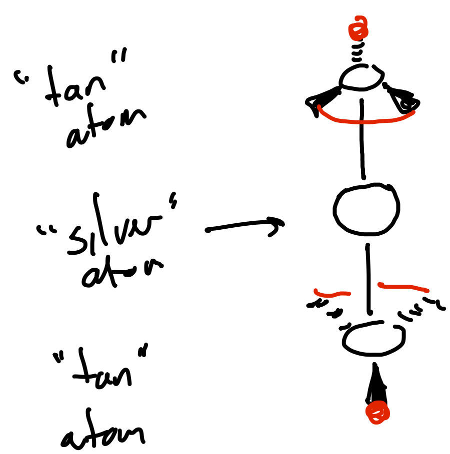


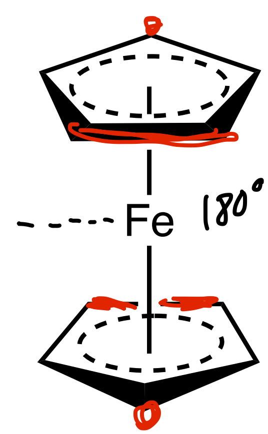
C_2

Used simplified structures



C_5

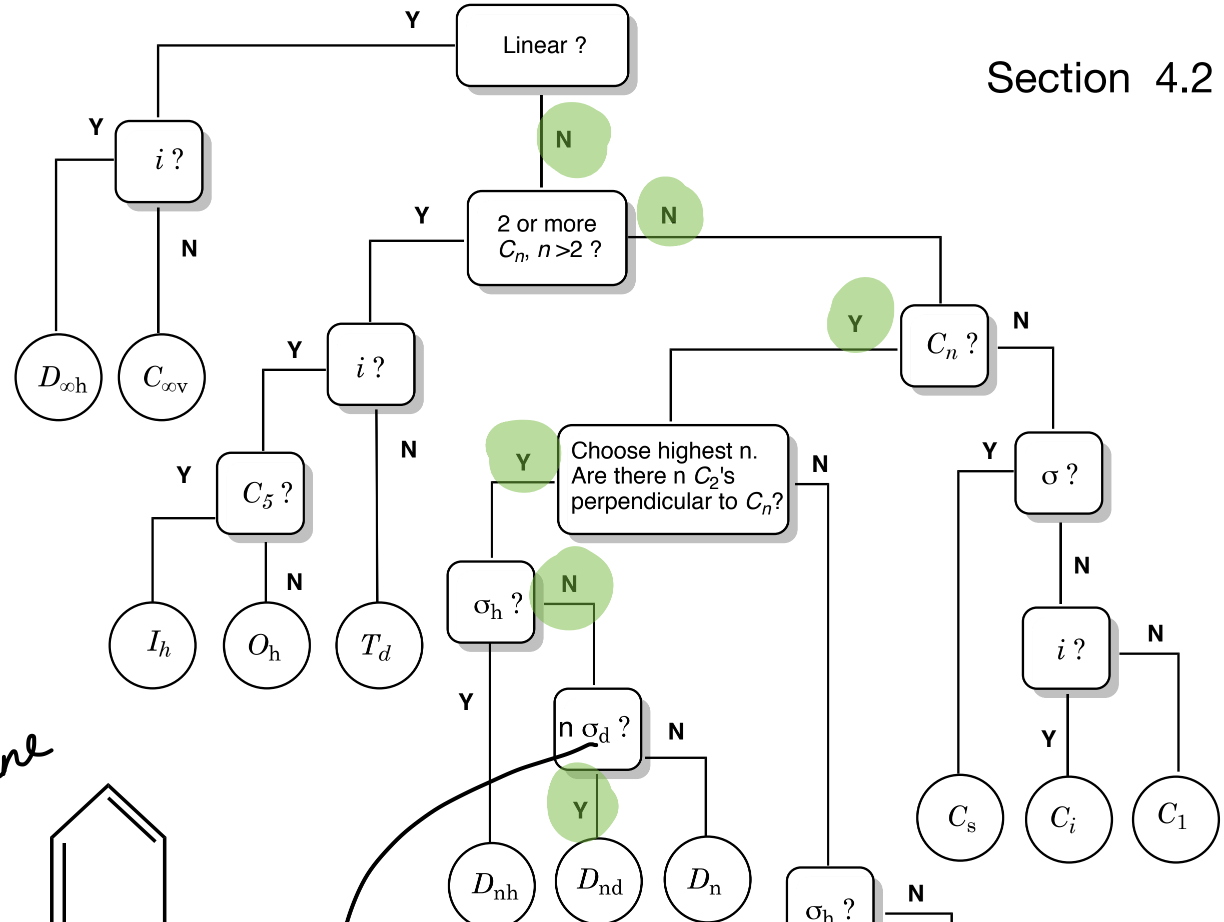
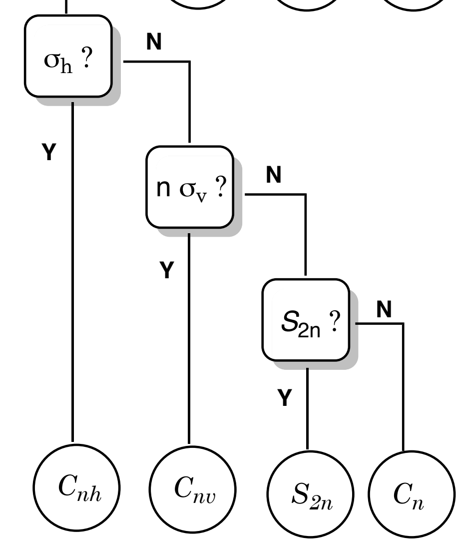


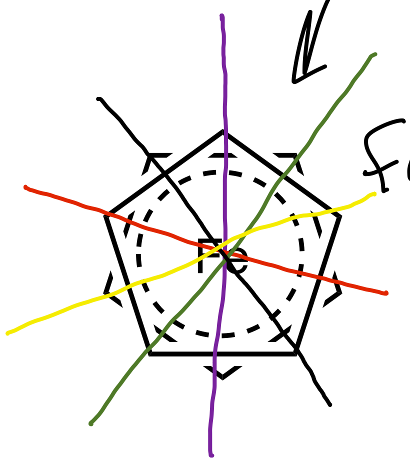


σ_v
σ_v

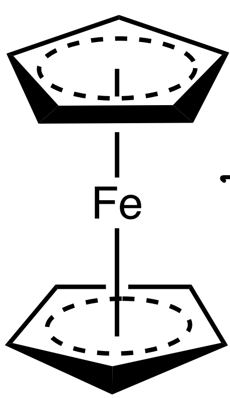
Practice

CH_2Cl_2
PCl_3
HCN
$PtCl_4^{2-}$ (square planar)
Fc
C_2H_2
H_2O
BrF_5
PPh_3

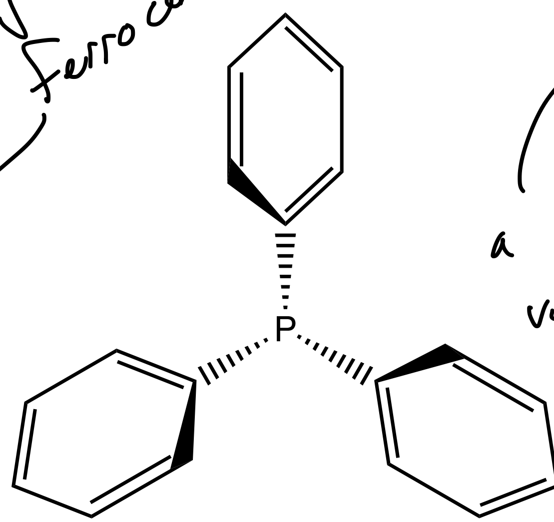





Find the pt group for Ferrocene



D_{5d}



a special kind of vertical σ

horizontal mirror planes are ⊥ to the principle axis

C_n with highest n

CH_2Cl_2	C_{2v}	Fc	D_{5d}
PCl_3	C_{3v}	BrF_5	C_{4v}
HCN	$C_{\infty v}$	PPh_3	C_3
$PtCl_4^{2-}$	D_{4h}	H_2O	C_{2v}
C_2H_2	$D_{\infty h}$		

In mathematics, a group is a **set** combined with an **operation** that has the specific mathematical properties properties

the operation combines any two elements of the set to form a third element which is part of the original set

other ways of saying this:
a set must be closed under the operation
there must be closure with respect to the operation

operating on elements of the set must satisfy the associative property

there must be an identity element in the set that when operated on by the operation along with any element of the set returns the original element

the operation in the set must be invertible; that is, the set must contain elements such that the operation on two elements in the set produce the identity element

It is a collection of symmetry operations with at least one fixed point that satisfies the criteria of being a mathematical "group"

C_{2v}

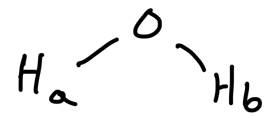
The set is the set of symmetry operations.
The operation is the symmetry operations operating on each other.

$$C_2 \text{ x } \sigma_{v(xz)} = \sigma_{v(yz)} \qquad C_2 \text{ x } \sigma_{v(yz)} = \sigma_{v(xz)} \qquad \sigma_{v(xz)} \text{ x } \sigma_{v(yz)} = C_2$$

$$C_2 \text{ x } (\sigma_{v(xz)} \text{ x } C_2) = \sigma_{v(xz)} \qquad (C_2 \text{ x } \sigma_{v(xz)}) \text{ x } C_2 = \sigma_{v(xz)}$$

$$E \text{ x } C_2 = C_2$$

$$C_2 \text{ x } C_2 = E$$



C_{2v}

E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$

(x, y, z)

Matrix representations

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

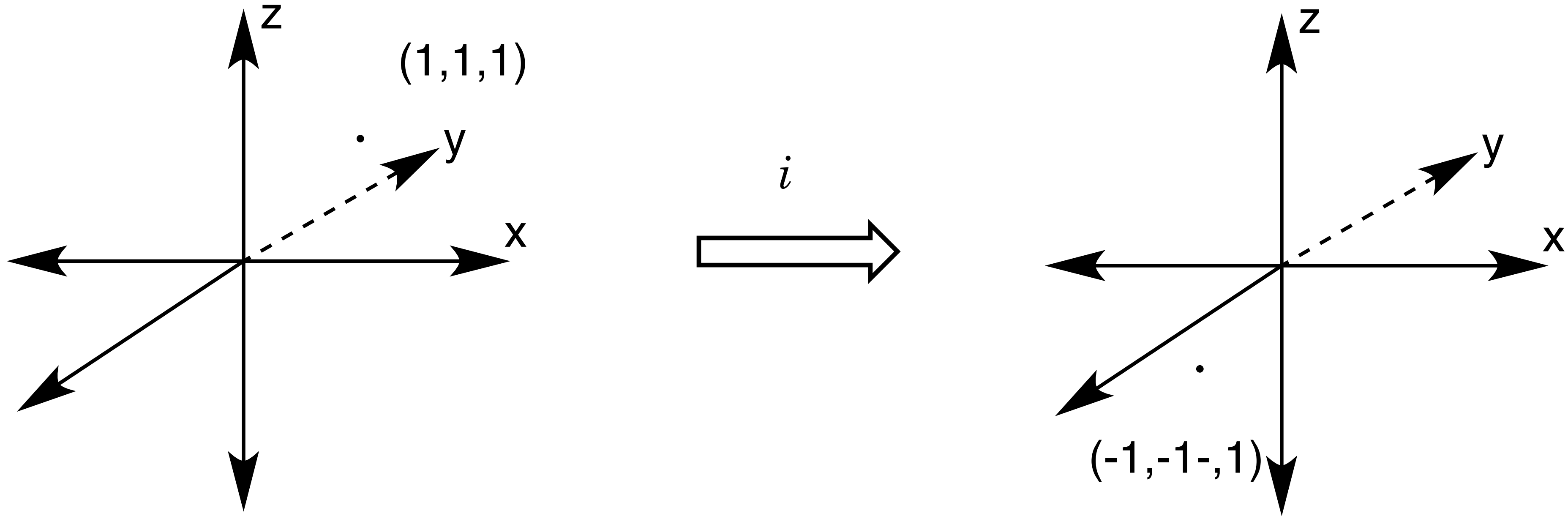
1x1 transformation matrices for each individual axis

1	-1	1	-1	x
1	-1	-1	1	y
1	1	1	1	z

The traces of the 3x3 transformation matices

3	-1	1	1

Transformation Matrices



$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \qquad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Matrix Multiplication…

Number of columns in the first matrix must equal number of rows in the second

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

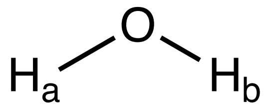
new x value = sum of Row 1 x Column 1

new y value = sum of Row 2 x Column 1

new z value = sum of Row 3 x Column 1

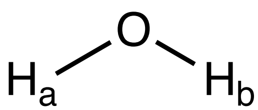
$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1(x) + 0(y) + 0(z) \\ 0(x) + -1(y) + 0(z) \\ 0(x) + 0(y) + -1(z) \end{bmatrix}$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ -z \end{bmatrix}$$

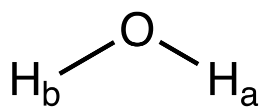


C_{2v} operations: E, C_2, $\sigma_v(xz)$, $\sigma_v(yz)$

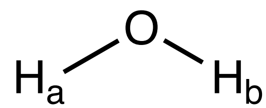
E



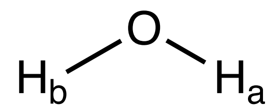
C_2



$\sigma_v(xz)$



$\sigma_v(yz)$



Matrix representations

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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

1x1 transformation matrices for each individual axis in the C_{2v} point group

1	-1	1	-1	x
1	-1	-1	1	y
1	1	1	1	z

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_{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

A Symmetric w.r.t. principle axis
B antisymmetric w.r.t. principle axis
subscript 1 is for representations that are symmetric w.r.t. a C_2 that is perpendicular to the principle axis
subscript 2 is for representations that are antisymmetric w.r.t. a C_2 that is perpendicular to the principle axis
in the absence of a C_2 a vertical mirror plane perpendicular to the plane of the molecule is used instead
subscript g symmetric w.r.t. inversion
subscript u antisymmetric w.r.t. inversion
' symmetric w.r.t. σ_h
'' antisymmetric w.r.t. σ_h