GROUP THEORY

1. Element of symmetry
2. Calculation of elements,
3. Point groups
4. Application of elements on axis x, y, z and matrix of each element.
5. **Representation :**
   1. Reducible
   2. Irreducible
   3. Derivation of character table.
6. **Application :**
   1. **Hybridisation :** For mixing of orbital having same symmetry and having same energy.
   2. IR/ Raman/ Microwave are also explained by group theory.

SYMMETRY :

Some tools for defining the symmetry like.

1. **Symmetry Elements :**There are 3 elements:

   (i) axis of symmetry
   (ii) Plane of symmetry
   (iii) centre of symmetry

Elements of symmetry	Operation of symmetry elements
Axis of symmetry	Rotation C_n operation
Plane of symmetry	Reflection. σ operation.
Improper axis of symmetry	Rotation -Reflection. S_n operation
Centre of Symmetry	Inversion (i)
Identity	Nothing to do for E

ELEMENT OF SYMMETRY :

Geometrical entity on the basis of that we can define the symmetry of an object is known as element of symmetry like, Axis, Plane, Point, etc.

OPERATION OF SYMMETRY ELEMENT :

Operation of symmetry element is the process which we apply on the element to define the symmetry.

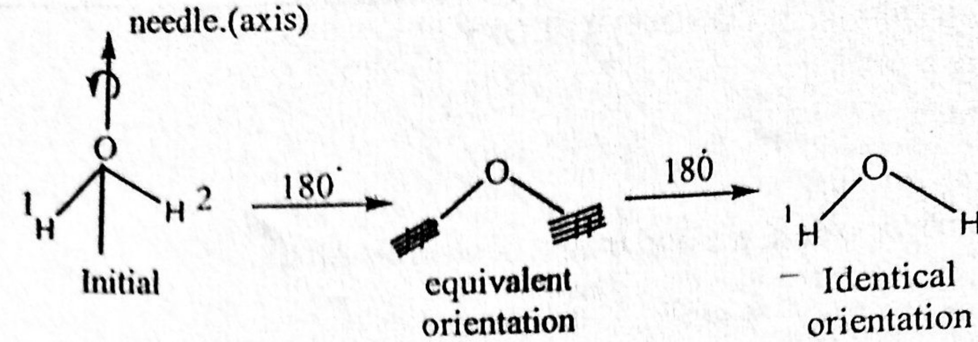
1. **Axis of Symmetry :**

Imaginary axis passing through the molecule rotation on which by θ^0 gives an equiva lent orientation.

Orientation of Molecule : 3D distribution of atoms of the molecule is called orientation two type of orientation of molecule.

(i) Identical Orientation :

The orientation of initial molecule through the equivalent orientation by which we get the same or exact identical molecule representation.



(ii) Equivalent Orientation :

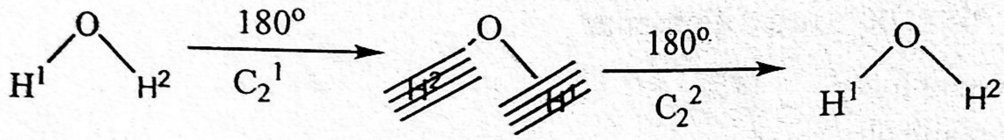
C_n OPERATION :

$$n = \frac{360}{\theta} = \frac{360}{180} = 2$$ Order of axis - C_2 axis

NUMBER OF OPERATION :

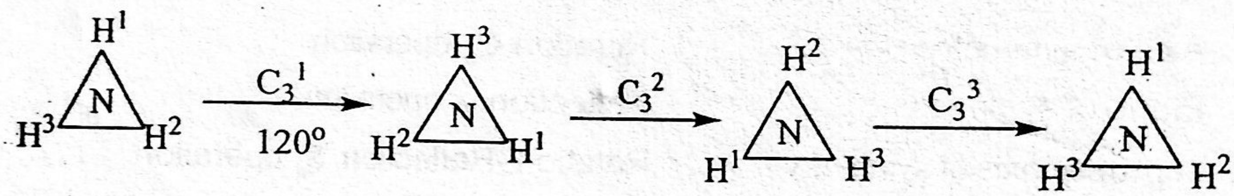
Number of operation to find the identical orientation (identity) . i.e.

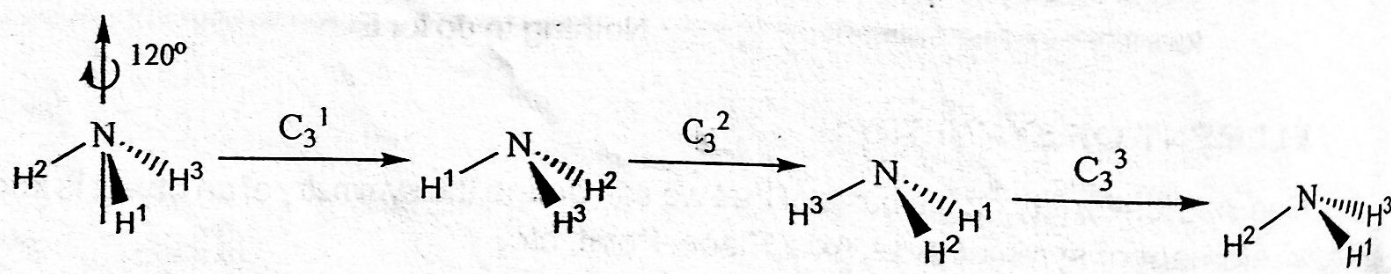
H_2O :



So the no. of operation = 1(because $c_2^2 = E$):

Example: NH_3 :



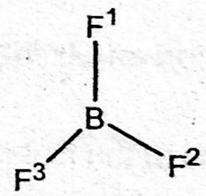


Order of axis = $\frac{360}{120} = 3 \rightarrow$ C_3 axis

Number of operation = 2 because C_3^3 is identity.

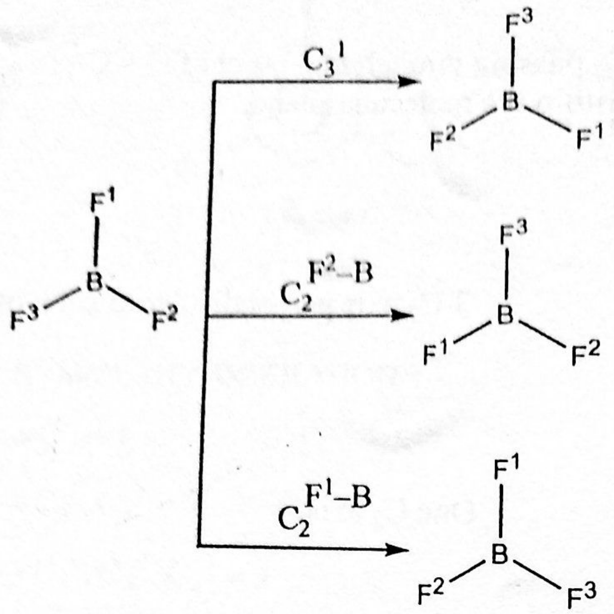
Example: BF_3 : 3 C_2 axis and 1 C_3 axis.

3 C_2 axis :

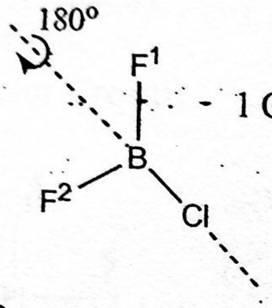


1. C_2 axis passing through $F^1 - B$ bond and interchanging F^2/F^3.
2. C_2 axis passing through F^2–B bond and interchanging F^1/F^3.
3. C_2 axis passing through F^3–B bond interchanging F^1/F^2.

1C_3 AXIS : C_3 axis passing through B atom and ⊥ to each C_2 axis.

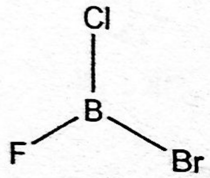


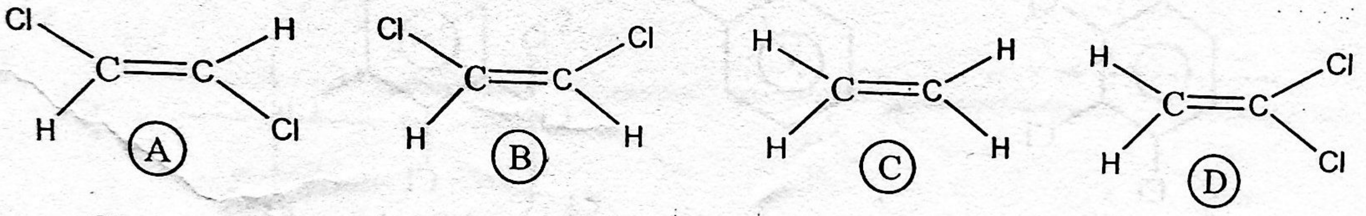
BF_2Cl :

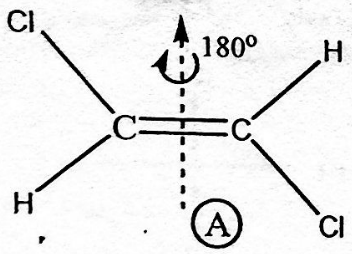


1 C_2 axis passing through B – Cl bond interchanging F^1/F^2.

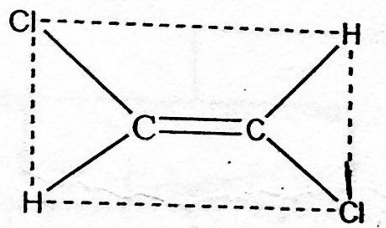
BFClBr :



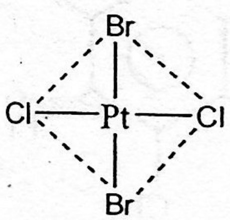




1 C_2 axis passing through double bond of carbon or mid point of C=C ⊥ to molecular plane



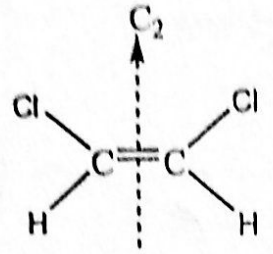
Rectangle



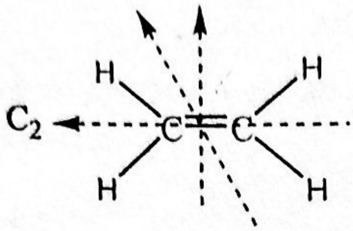
Square

C_2 is not present at diagonal in rectangle structure.

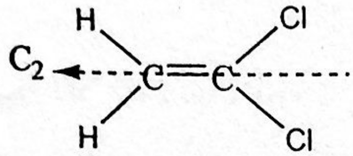
C_2 present at diagonal in square planar structure



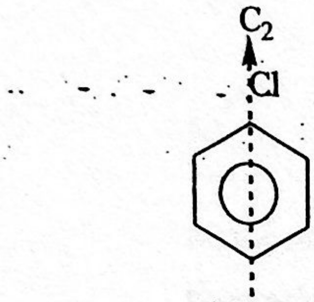
C_2 passing through mid point of C = C within the molecular plane.



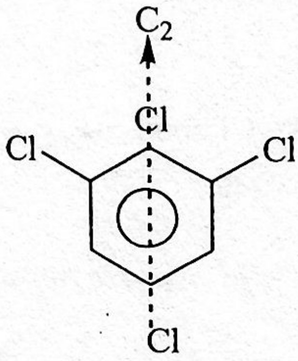
3 C_2 axis perpendicular to each other



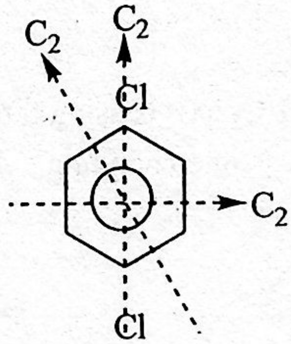
One C_2 axis.



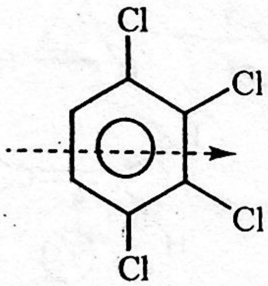
1 C_2 axis.



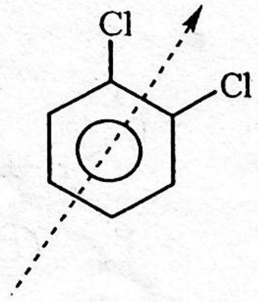
1 C_2 axis.



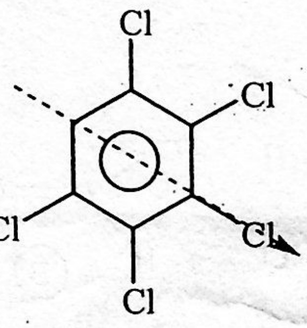
3 C_2 axis.



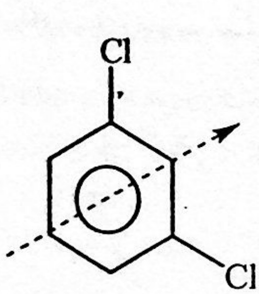
1 C_2 axis.



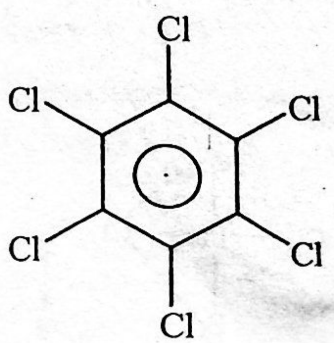
1 C_2 axis.



1 C_2 axis.

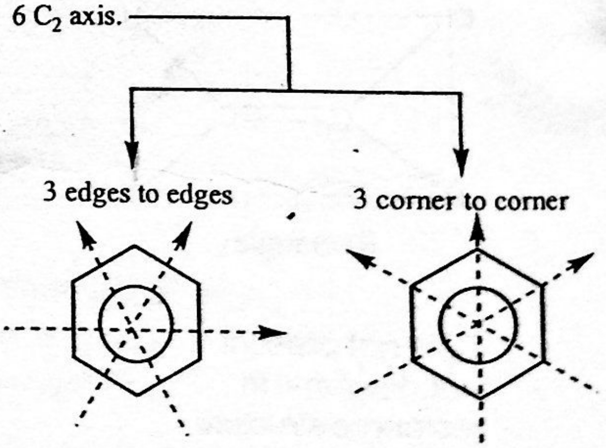


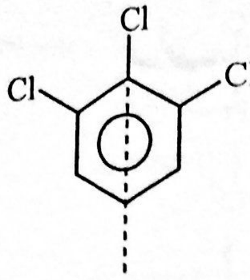
1 C_2 axis.



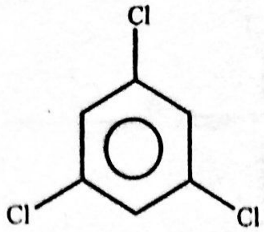
1 C_6 axis.

6 C_2 axis.



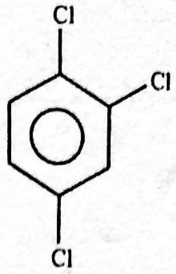


1 C_2 axis.



1 C_3 axis.

3 C_2 axis



No axis

NUMBER OF SYMMETRY OPERATION :

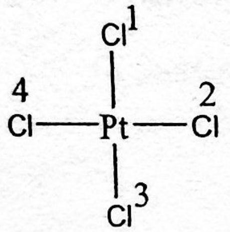
$$C_2 \longrightarrow C_2^1 = 1$$

$$C_3 \longrightarrow C_3^1, C_3^2 = 2$$

$$C_4 \longrightarrow C_4^1, C_4^2, C_4^3 = 3$$

$$C_5 \longrightarrow C_5^1, C_5^2, C_5^3, C_5^4 = 4$$

D_{4h} Point Group:



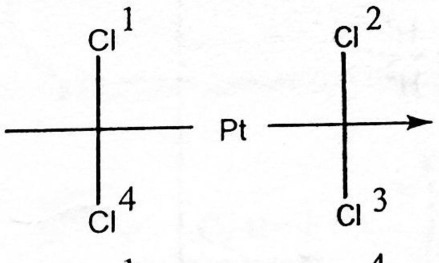
$K_4 + 4C_2$

4 C_2 axis.

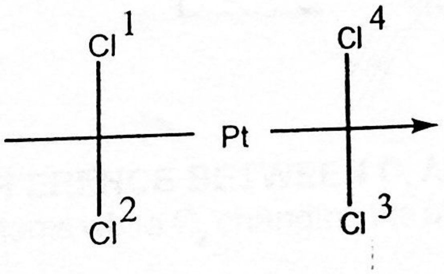
C_2 passing through $Cl^1 - Pt - Cl^3$

C_2 passing through $Cl^2 - Pt - Cl^4$

C_2



C_2

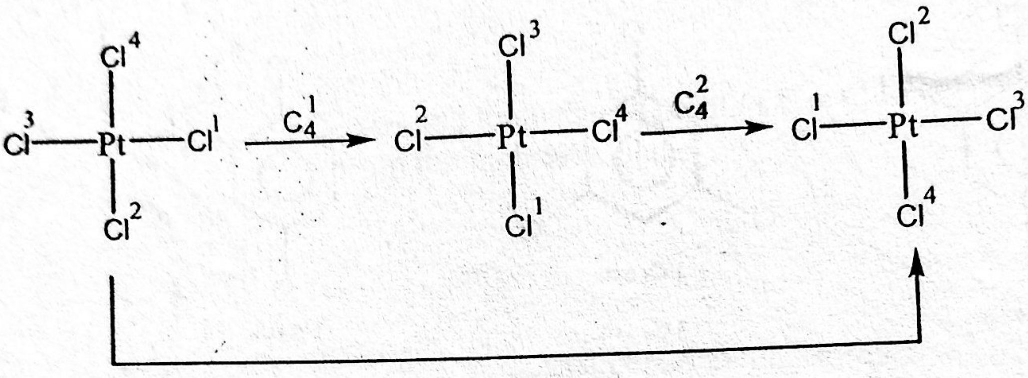


1C_4 AXIS : C_4 passing through Pt ⊥ all C_2 axis

C_4^1 $\quad$ C_4^2 $\quad$ C_4^3

$\|$

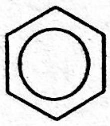
C_2 axis



$180^o = C_2$

$C_4^2 = C_2$

C_6^1 C_6^2 C_6^3 C_6^4 C_6^5



$C_6^2 \rightarrow C_3$ (120°)

$C_6^3 \rightarrow C_2$ (180°)

$C_6^4 \rightarrow C_3$ (120°)