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M. Sc. Chemistry Semester –I

Inorganic chemistry Lect : 2

- **Point Group of molecules**
- **Classification of Point group**

Point group :

- It is a collection of all the symmetry operation that can be carried out on the molecule is called as point group.

- It is a short hand notation which gives an information about the number of operation that can be carried out on the molecules.

- Point group must satisfy the properties of group and also used for the storing the information regarding the structure of molecule.
- In a point group, all symmetry elements must pass through the center of mass (the point).

- General notation of point groups : C_s, C_1, C_i, C_n, C_{nv}, C_{nh}, D_n, D_{nh}, D_{nd}, T_d, O_h, $C_{\infty v}$, $D_{\infty h}$

Classification of Point group

1. **Molecules of low symmetry**
2. **Molecules of high symmetry**
3. **Molecules of special symmetry**

1. Molecules of low symmetry :

Least number of symmetry elements possessed by geometrical molecules. Generally molecules the molecules has e highly unsymmetrically substituted atoms

It includes C_1, C_s, C_i point group

C_1 Point group : The molecules contains only E element and other elements of symmetries are absents . Such molecules possesses highly unsymmetrically substituted atems

Ex. Tetrahedral CHClBrI , Square pyramidal NbF_7

C_s Point group : The molecules contains only E and σ plane and other elements of symmetries are absents .

Ex. Phenol, Aniline,

C_i Point group : The molecules contains only E and i center of inversion and other elements of symmetries are absents .

Ex. Trans $C_2H_2F_2Cl_2$

2. Molecules of high symmetry :

C_n Point group : The molecules contains only E and C_n rotational axis and other elements of symmetries are absents .

- Ex. PPh_3, - C_3 point group (E, C_3 axis)
  PPh_3 - C_3 point group (E, C_3 axis)

C_{nv} Point group : The molecules contains only E , C_n axis and $n\sigma_v$ planes .

❖ Ex. Draw the structure and label the possible element of symmetry and identify the point group of the following molecules

❖ H_2O - C_{2V}

❖NH_3 - C_{3V}

❖$POCl_3$ - C_{3V}

❖T Shaped ClF_3 – C_{2V}

❖Square pyramidal WOF_4 - C_{4V}

C_{nh} Point group : The molecules has E , C_n axis, center of inversion 'i' and σ_h planes perpendicular to principal axis .

❖ Ex. Draw the structure and label the possible element of symmetry and identify the point group of the following molecules

❖ trans 1,2 dichloro ethylene - C_{2h}

❖ $B(OH)_3$ - C_{3h}

D_n Point group : The molecule contains C_n axis and nC_2 perpendicular to C_n axis .

$Dn = C_n + nC_2 \perp C_n$

❖

D_{nh} Point group : The molecule contains C_n axis and nC_2 perpendicular to C_n axis and C_n perpendicular σ_h

$D_{nh} = C_n + nC_2 \perp C_n \quad + C_n \perp \sigma_h$

Draw the structure and label element of symmetry and identify point group of the following molecules

- BF_3, CO_3^{--}, PCl_5 – D_{3h} point group
- $[PtCl_4]^{--}$, trans $[CoCl_2(NH_3)_4]^+$ - D4h point group
- C_5H_5- -D_{5h} point group
- C_6H_6 – D_{6h} point group
- Eclipsed $Fe(C_5H_{5)2}$ -D_{5h} point group

D_{nd} Point group : The molecule contains C_n axis and nC_2 perpendicular to C_n axis and C_n perpendicular σ_h

$D_{nh} = C_n + nC_2 \perp C_n \quad + C_n \perp \sigma_d$

Draw the structure and label element of symmetry and identify point group Staggered confirmation $Fe(C_5H_5)_2$ - D_{5d}

3. Molecules of Special Symmetry :

$C_{\infty v}$ Point group : heteronuclear diatomic molecules contains C_∞ axis and $\infty\ \sigma_v$ plane and other elements of symmetries are absents .

- Ex : HCl, CO, NO CN, HCN - **$C_{\infty v}$** point group

$D_{\infty h}$ Point group : The molecule contains C_∞ axis and ∞C_2 perpendicular to C_∞ axis and C_∞ perpendicular σ_h

$D_{\infty h} = C_\infty + \infty C_2 \perp C_\infty + C_\infty \perp \sigma_h$

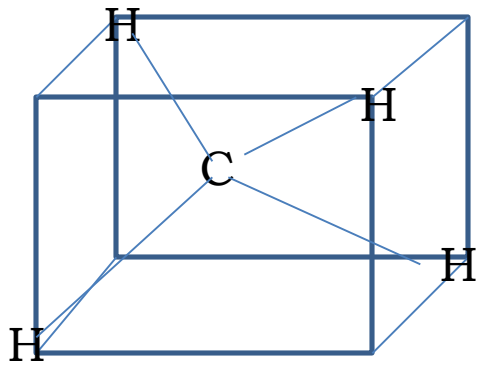
Draw the structure of following molecules and lable element of symmetry and identify the point group Cl_2, H_2, CO_2, **$D_{\infty h}$** point group

4. Molecules containing multiple higher order of axes:

T_d Point group : Symmetrical tetrahedral molecules has multiple order rotational axis

Ex : CH_4, $SiCl_4$, $TiCl_4$, **T_d** point group

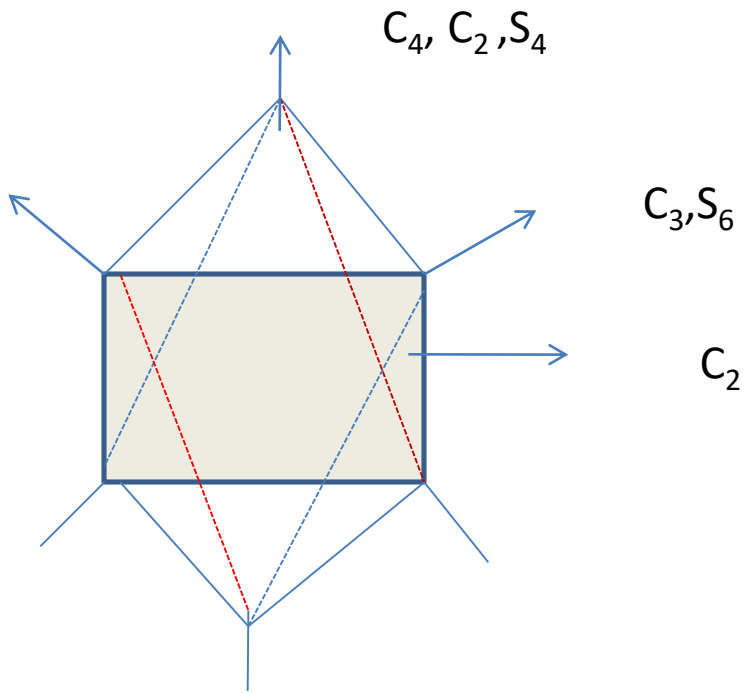
T_d= (E, $4C_3^1$, $4C_3^2$, $3C_2^1$, $3S_4^1$, $3S_4^3$, 6 σ_d) order of group is 24



O_h Point group : Symmetrical octahedral molecule has multiple order of rotational axis and has O_h point group

- Ex : FeF_6, AB_6

O_h= (E, $3C_4^1$, $3C_4^2$,$3C_4^3$, $6C_2^1$, $4C_3^1$, $4C_3^2$ $3S_4^1$, $3S_4^3$, $4S_6^1$, $4S_6^5$, i, $3\sigma_h$,$6\sigma_d$) order of group is 48



Molecules	**Symmetry elements in the groups**	**h**	**Point Group**
CFClBrI	E,	1	C_1
HOCl	E, σ	2	C_s
Trans-CHFCl-CHFCl	E, i	2	C_i
Cis- H_2O_2	E, C_2	2	C_2
H_2O, H_2S, SO_2	E, C_2, $2\sigma_v$	4	C_{2V}
NH_3	E, C_3^1, C_3^2, $2\sigma_v$	6	C_{3V}
SF_5Cl	E, C_4^1, $C_4^2 = C_2^1$, C_4^3 $4\sigma_v$	8	C_{4V}
HCl	E, , $C_{2\infty}$, $\infty\sigma_v$	∞	$C_{\infty V}$
Trans-$C_2H_2Cl_2$	E, C_2, i,σ_h	4	C_{2h}
Tran – $Pt(NH_3)_2Cl_2$	E, C_2, $2C_2'$, $2\sigma_v$, i, σ_h	8	D_{2h}
BF_3	E, C_3^1, C_3^2, $3C_2^1$, $3\sigma_v$, σ_h, S_6^1, S_6^5	12	D_{3h}
	E, C_4^1, $C_4^2 = C_2^1$, C_4^3 , $4C^{21}$, $2\sigma_v$, $2\sigma_d$, σ_h, , i, S_4^1, S_4^5	16	D_{4h}
C_6H_6	E, , $C_{2\infty}$, $\infty\sigma_v$, σ_h, i	∞	$D_{\infty h}$
CH_4	E, $4C_3^1$, $4C_3^2$, $3C_2^1$, $3S_4^1$, $3S_4^3$, 6 σ_d	24	T_d
FeF_6	E, $3C_4^1$, $3C_4^2$,$3C_4^3$, $6C_2^1$, $4C_3^1$, $4C_3^2$ $3S_4^1$, $3S_4^3$, $4S_6^1$, $4S_6^5$, i, $3\sigma_h$,$6\sigma_d$	48	O_h

THE END