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CSIR–NET

Chemical Science

Council of Scientific & Industrial Research (CSIR)

Volume - 1

Inorganic Chemistry

SIERRA INNOVATIONS

INDEX

2 CHAPTER

Chemical Bonding

Que. What is chemical bond?

Ans. Force of attraction between two atoms.

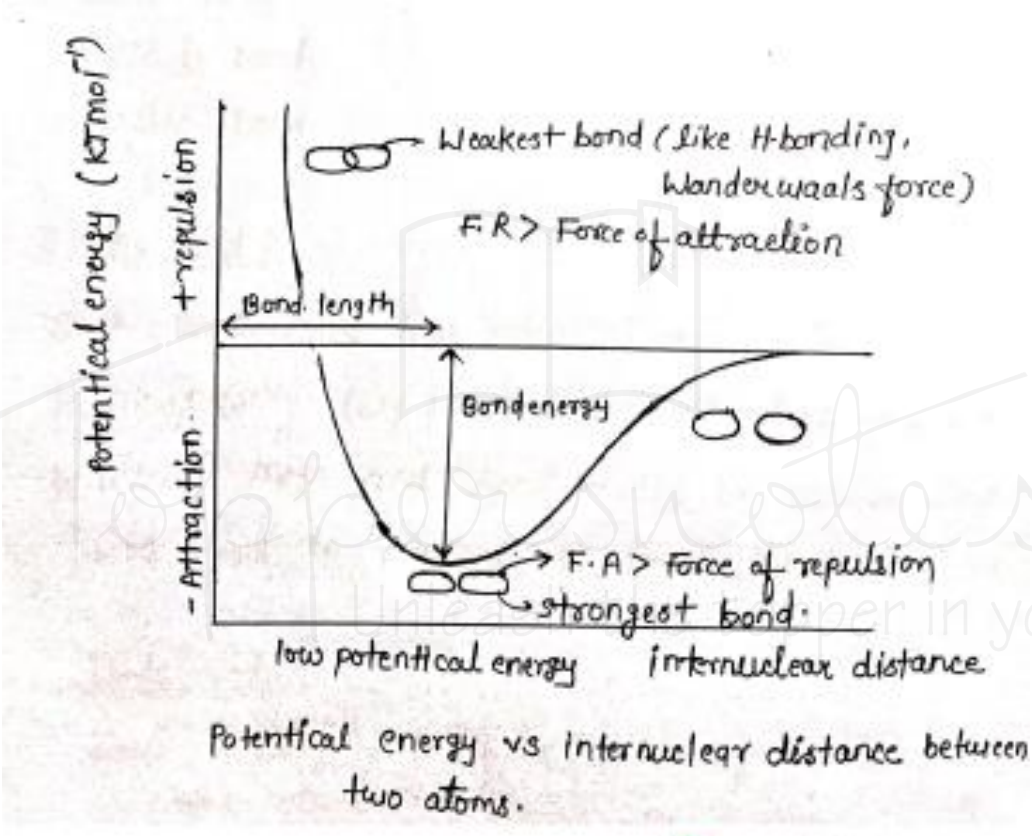
When Force of attraction > Force of repulsion → **bond form.**

Force of repulsion > Force of attraction → **bond does it form.** (Note: intended "does not form")

Que. Why a chemical being is formed?

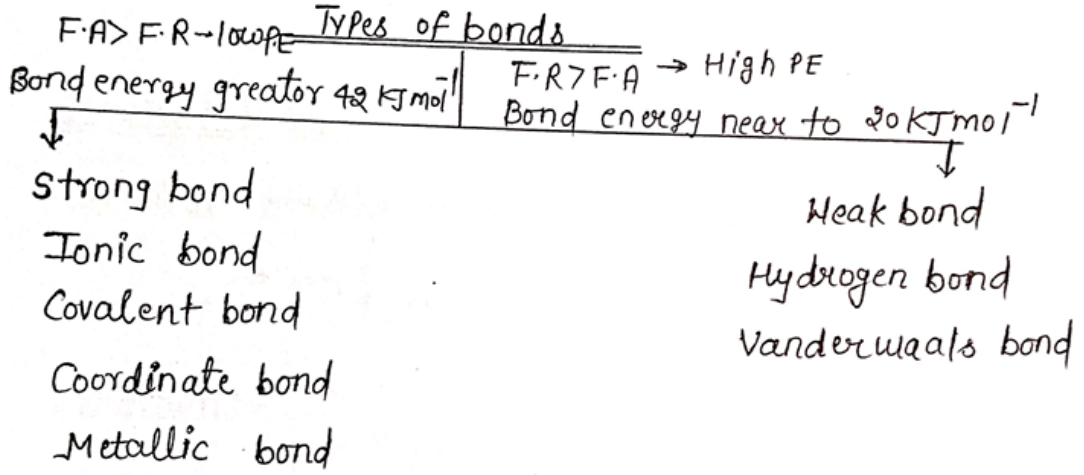
Ans. To achieve the stability.

Force of attraction > Force of repulsion



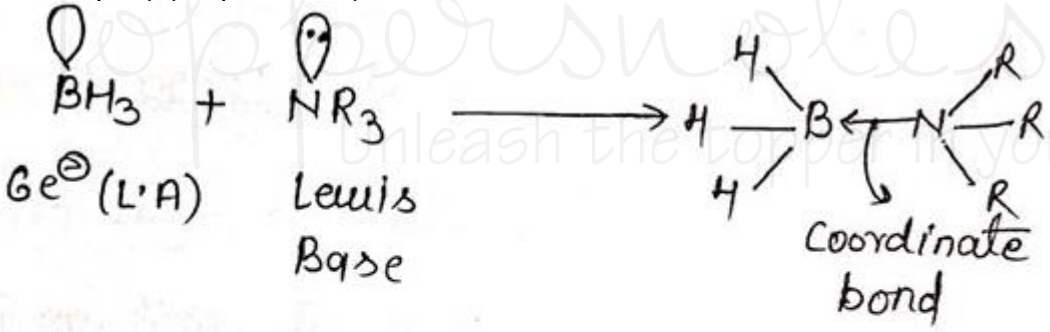
Potential energy vs internuclear distance between two atoms.

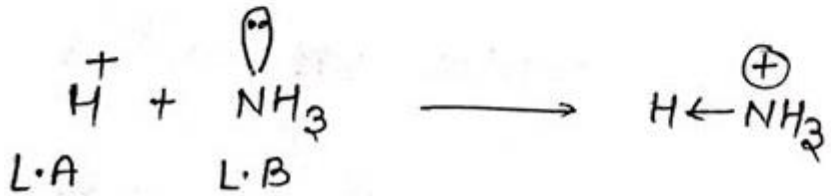
- Low potential energy → strongest bond → Force of attraction > F.R
- High potential energy → weakest bond → F.R > F.A



- **Strong Bond:-**
  - ✓ Such bonds have low potential energy and thus High stability they have strong attractive forces between them and bond energy is greater than 42 kJ / mol is required to break the bond.
- **Ionic Bond:-**
  - ✓ Ionic bonding is the complete transfer of valence e^- b/w atoms.
  - ✓ Metal + Non-Metal → Ionic bond
    (electro +ve element) + (electro -ve element)
  - ✓ $Na + Cl \rightarrow Na^+Cl^-$
    $2p^6 3s^1\ 3s^2 3p^5$
  - ✓ $2Ca + Cl_2 \rightarrow CaCl_2$ $(+2, -2$ charges)
- **Covalent bond:-**
  - ✓ Chemical bonding is the sharing of e^- between atoms.
    $H \cdot + \cdot H \rightarrow H - H$
- **Condition:-**
  - ✓ Both elements are non-metal formation of covalent bond.
  - ✓ Electro -ve element + electro -ve element → covalent bond
  - ✓ **Ex.** $F \cdot + \cdot F \rightarrow F - F$
  - ✓ **Ex.** $H \cdot + \cdot Cl \rightarrow HCl$
- **Coordinate bond / Dative bond:-**
  - ✓ A coordinate bond is a type of covalent bond but
  - ✓ But in this bond the electrons are shared by a single atom, whereas the second atom accepts the electrons.

    Lewis acid + Lewis Base → Coordinate bond
    (e^- pair acceptor) (e^- pair donor)

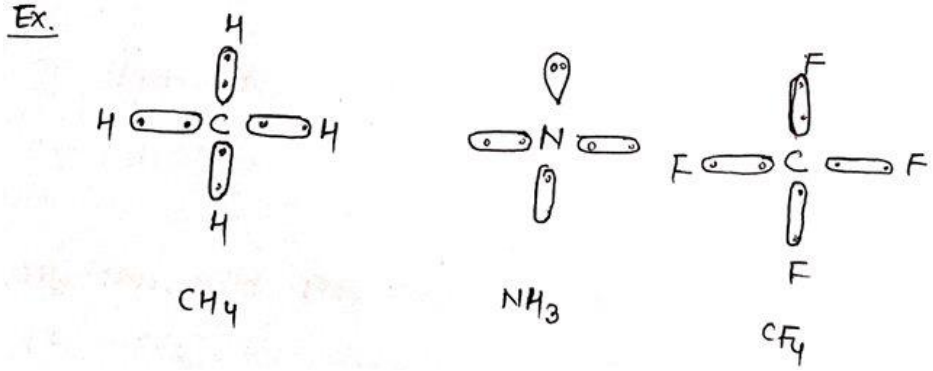




- **Metallic Bond:-**
  - ✓ Metallic bond force that holds atom together in a metallic substance. Such a solid consists of closely packed atom. In most cases the outermost e^- shell of each of the metal atoms overlap with a large number of neighbouring atom.

    $Fe - Fe$ (Metallic bond)
    $Mn_2(CO)_{10} + Na \rightarrow [Mn(CO)_5]^-$ (Weakest bond)
    (close packed) smaller size → good overlap → strong metallic bond
    larger size (not closed packed) → Bad overlap → weak metallic bonds
    Metallic bond is weaker than ionic, covalent, coordinate bond.

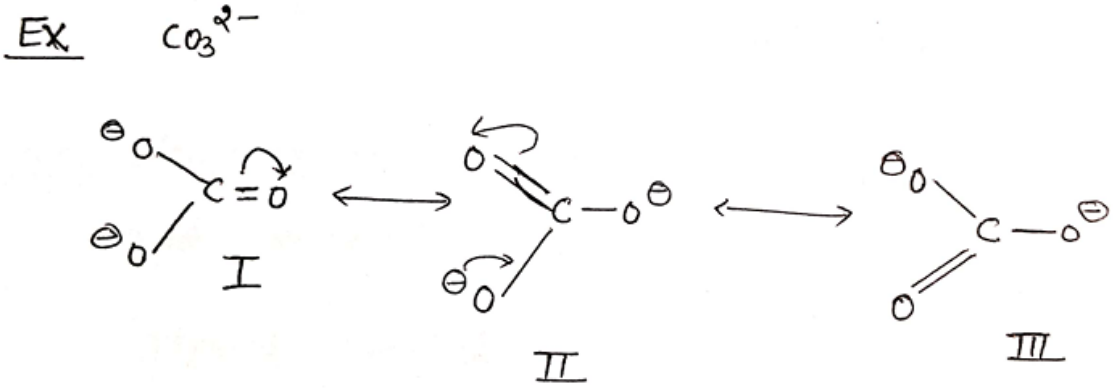
- **Lewis Octet Rule:-**
  - ✓ According to this rule an atom undergoes bond formation in order to complete its octet i.e. 8 e^- in the valence.



  - ✓ But all molecules does not follow octet rule.
    - **(i) Hypovalent species:-**
      - Less than 8 e^- called Hypovalent species.
      - **Ex.** BF_3 BCl_3, BI_3, BH_3, $AlCl_3$
    - **(ii) Hypervalent species:-**
      - More than 8 e^- called Hypervalent species.
      - **Ex.** PCl_5, PF_5, SF_6, XeF_6
  - ✓ Generally 2nd period elements follow octet rule but 3rd or 4th period elements does not follow octet rule because they shows expanding.

- **Condition for expanding:-**
  - ✓ If Central atom containing vacant d-orbital.
  - ✓ Electronegativity of surrounding atom must be more than hydrogen.
  - ✓ If Hydrogen is surrounding atom they are not expanding.
  - ✓ $OH_2, NH_3, NCl_3, PCl_3, PCl_5, PF_3, PF_5, SF_6, XeF_6$ are exist
  - ✓ $PH_3 \rightarrow PH_5$ (Not exist)
  - ✓ $SH_4 \rightarrow SH_6$ (Not exist)
  - ✓ $XeH_4 \rightarrow XeH_6$ (Not exist)
  - ✓ Because surrounding atom is hydrogen.
  - ✓ PH_5 (2.1 EN) → $3s^2 3p^3 3d^0$ but (more distance less attraction)
  - ✓ PF_5 (4.1 EN) → $3s^2 3p^3 3d^0$ (s or d → less distance more attraction)

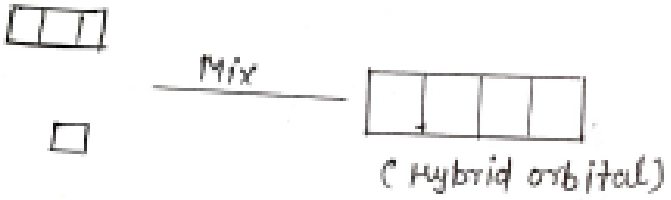
- **Bond order:-**
  - ✓ Bond order of the molecule giving several resonating structure is calculated using the formula given below.
  - ✓ **Average bond order** = (Total no. of bonds formed between any 2 atom in all the structure) / (Total no. resonating structure.)

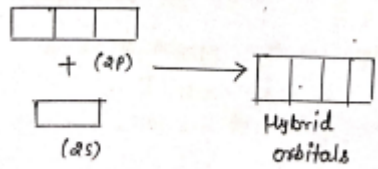
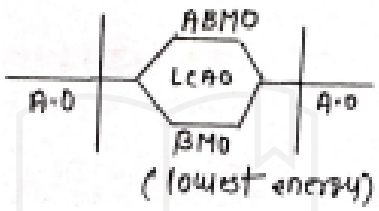


$$\text{Bond order} = \frac{\text{No. of atoms}}{\text{resonating str.}}\ (3\sigma + 1\pi) = \frac{4}{3} = 1.33$$

This formula only applicable for trigonal planer molecule.

- **Valence bond theory (VBT):-**
  - ✓ VBT used for find out Hybridisation of molecule. This theory says that a covalent bond between two atoms is formed when atomic orbitals of proper energy and symmetry overlaps. Heitler and London proposed this theory and later on Pauling and Slater extended it.



Hybrid orbital	Molecular orbital
When two orbitals of same energy mix together, hybrid orbitals are formed.	When in a molecular orbital, two orbitals of the same energy overlap they form either a bonding molecular orbital or an antibonding molecular orbital.
	

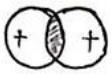
Que: Among s-s, p-p and s-p which has the longest bond length?

Ans: Heitler and London could not explain this concept. It was explained by Pauling and Slater.

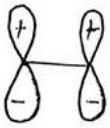
- **According to Heitler and London:-**
  - ✓ Two atoms must come close to one another so that the overlapping of orbital of one atom with the orbital of other atom could take place.
  - ✓ For the formation of a covalent bond.
    $H \curvearrowleft\curvearrowright H \rightarrow H - H$
  - ✓ For the formation of bond electron must have unpaired or antiparallel.
    $H \curvearrowleft\curvearrowright H \rightarrow H - H$
  - ✓ Wherever the attraction is greater (bond is stronger) the bond energy will be higher but the bond length will decrease.
    Ex. H-F, HCl, H-Br, HI
  - ✓ **Bond length order:** HF < HCl < HBr < HI
  - ✓ In HF Fluorine is more electronegative the bond energy is higher. Whereas in HI due to less attraction the bond energy is lower. So in HF compared to HI the bond length is shorter.
  - ✓ **Concept:** attraction ↑ Electronegativity ↑ Bond energy ↑ Bond length ↓

- **Extension by Pauling and Slater:-**
  - ✓ The extent of overlapping depends on the following factor.
    1. **Nature of the overlapping itself:-**
       - The smaller principal quantum number and closer it is the nucleus, overlapping will be better.

       n=1 (k-shell, good overlapping) n=3 (M-shell)
       n=2 (L-shell) n=4 (N-shell, weak overlapping)
    2. s-orbital have non-directional and spherical shape. s-orbital show headwise overlapping. but p-orbital have directional in nature and dumbel shape they show both types of overlapping head or lateral.

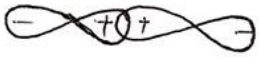


head on overlapping
gereade (g)



Head - Head overlapping

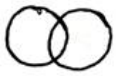
Presence of center of symmetry called gereade (g).



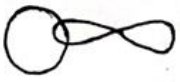
Side-wise overlapping
Absence of center of symmetry
Called ungerade (u).

Extended of overlapping :- 1s-1s > 2s-2s > 3s -3s

3. **d-orbital :-** Double dumbel shape and presence of center of symmetry called gereade.



S-S
σ-bond



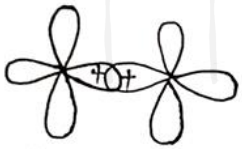
S-Pz
σ-bond

$sp^n - sp^n$
σ-bond

sp^n-s
σ-bond

Pz - Pz
σ-bond

$dz^2 - dz^2$
σ-bond

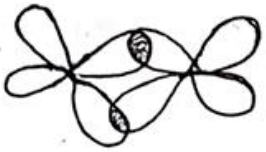


dx^2-y^2 dx^2-y^2

- ✓ In head-on overlapping sigma (σ) bond is always formed.
- ✓ In Π bond formation, sidewise overlapping always occurs.
- ✓ When during σ bond formation the signs are ++ or -- then a bonding molecular orbital is formed.
- ✓ When the signs are +- or -+ then an antibonding molecular orbital is formed.

Pπ-dπ bond
Formation

Pπ-dπ bond Formation
(2nd - 3rd)



dπ-dπ overlaping
π-bond Formation

- ➢ **Strength of bonds:-**
  - ✓ The bond strength of bonds between two orbitals depends on the following factor.

(A) Principal quantum Number (n):- Lesser the principal quantum number (n) of the orbital smaller is its size and stronger the bonds it forms.

Ex. Sigma bond formation occurs in both 1s-1s and 2s-2s overlap, but the bond strength is greater in 1s-1s than in 2s-2s because the size is smaller.

(B) Directional nature :- orbitals with directional nature show better overlapping as compared to non-directional orbitals.

$P_z + P_z \rightarrow \sigma$ but

$P_z \rightarrow$ directional $\rightarrow$ good overlapping

$s + s \rightarrow \sigma$ but $s \rightarrow$ Non directional $\rightarrow$ Bad or Weak overlapping

- ✓ Due to the spherical shape of the s-orbital, electron density can be present anywhere around the nucleus.

(3) % percentage s-character : If percentage of s-character ↑ strongest bond will be form.

% s-character α bond strength α good overlapping

$sp > sp^2 > sp^3$

50% 33% 25%

More bond strength less bond length

Order of domination of different factor

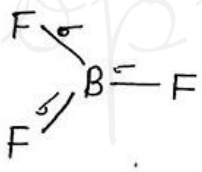
% age s character > principal quantum NO > Directional nature

Hybridisation: Atomic orbitals having the same energy mix to form the same number of hybrid orbitals.

σ bonds + lone pair = Electron pair (Hyb^n)

Π-bond does not participate in Hybridisation

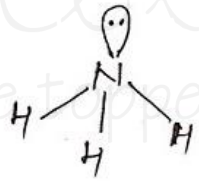
Ex BF_3



$3\sigma - B.P + 0L.P = 3EP$

$Hyb^n = sp^2$

Ex. NH_3



$3\sigma - B.P + 1L.P = 4EP$

$Hyb^n - sp^3$

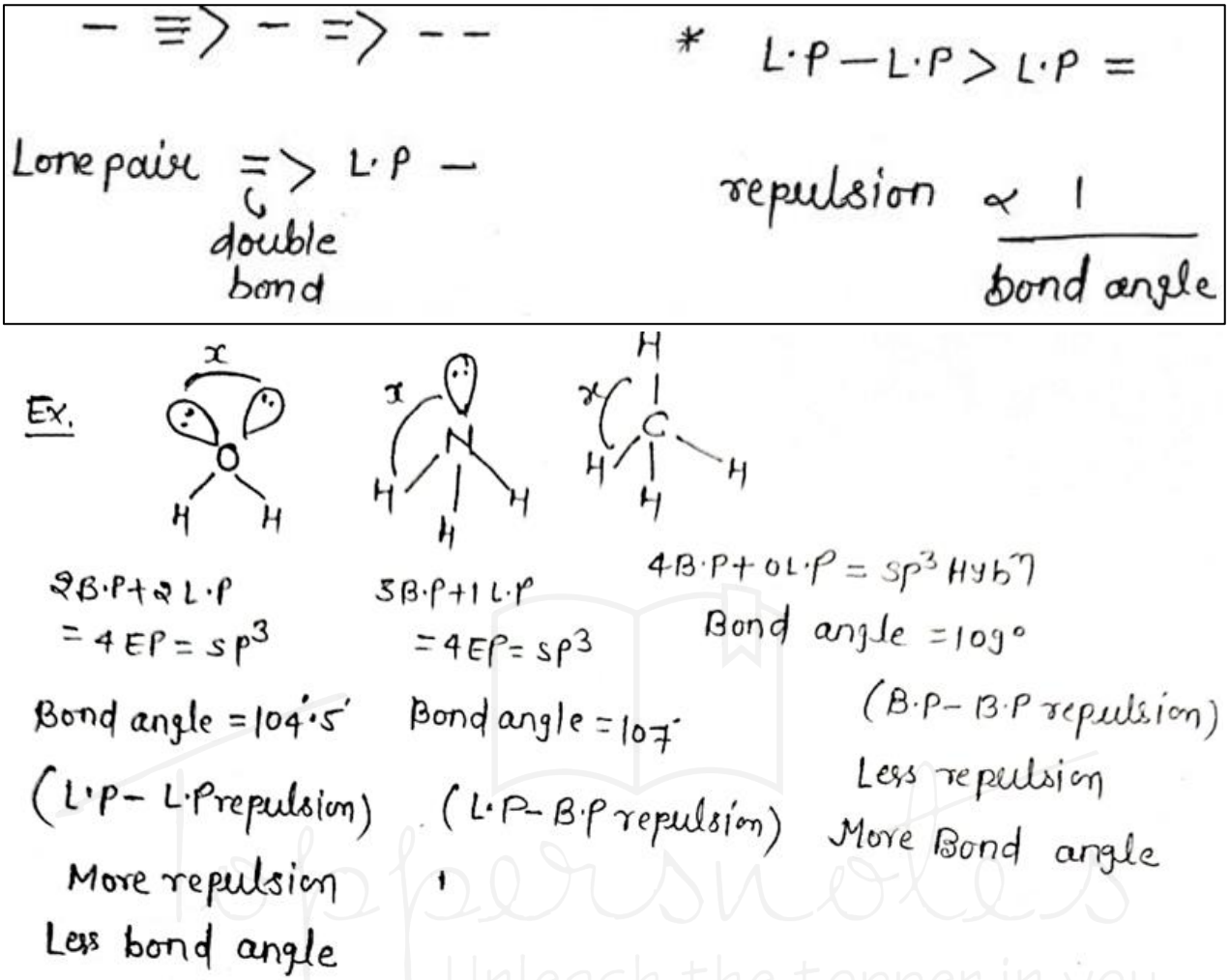
Electron pair	Hybridisation	Geometry	Bond angle
2 EP	sp	linear	180°
3 EP	sp^2	Trigonal planar	120°
4 EP	sp^3	Tetrahedral	109° 28°
5 EP	sp^3d	Trigonal bipyramidal	120° (eq-eq) 90° (axial-eq)
6 EP	sp^3d^2	Octahedral	90°
7 EP	sp^3d^3	P.B.P	90°/72°
8 EP	sp^3d^4	Sq. antiprismatic	45°

- ➢ **VSEPR Theory:**
  - ✓ VSEPR Theory applicable only for non-transition element (specially p-block)
  - ✓ VSEPR not applicable for transition element (3d/4d/5d)
  - ✓ VSEPR use for shape and geometry specially for P-Block elements.

- **VSEPR Theory:** Find out the shape and Hybridisation of non-transition element.
- **Repulsion Sequence:** Find out bond order and bond angle.

  [L.P - L.P > L.P - B.P > B.P - B.P]

  More repulsion less Bond angle Less repulsion more bond angle



- **STEP-1 Find out Central atom**
  - ✓ Less electronegative element is always central atom except Hydrogen.
    - Hydrogen is always present in the surrounding (terminal position) it can never act as a central atom.
    - Generally in a molecule the atom that appears only once (single atom) is the central atom.
    - Ex. NSF_3 : Here S is central atom
    - Ex. XeF_5 : Here Xe is central atom
    - Ex. IF_5 : Here I is central atom

- **Step II:** Find out the valence e^- of central atom.

G-I	G-II	G-13	G-14	G-15	G-16	G-17	G-18
ns^1	ns^2	ns^2np^1	ns^2np^2	ns^2np^3	ns^2np^4	ns^2np^5	ns^2np^6
valence 1 e^-	$2e^-$	$3e^-$	$4e^-$	$5e^-$	$6e^-$	$7e^-$	$8e^-$

- **Step-III: Find out the valency of surrounding atom:-**

G-I	G-II	G-13	G-14	G-15	G-16	G-17	G-18
valency 1	2	3	4	3	2	1	0/8

  - ✓ In Group 14, Group 15 and Group 16, those elements which have vacant d-orbitals can expand their octet so their valency also increases.
  - ✓ Ex. $PCl_5 \rightarrow$ Group 15 element. P = 5 valency (due to expanding)

- **Step-IV: Find out the electron pair**
  - ✓ Electron pair = No. of Bond pair + No. of lone pair

Ex. NSF_3 → S → surrounding atom

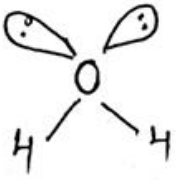
X – F
X – F
X – F
X
X
X N
X

= 4 + 0·LP = 4EP

Hybⁿ = sp^3

- **Step-V: Find out geometry and shape.** Geometry = With lone pair = No. of B.P + L.P shape = Without lone pair = No. of only bond pair (σ bond)

Ex.



4 EP = sp^3 Hybⁿ

Geometry = Td

shape = V-shape / bent shape / Angular shape

  - ✓ In VSEPR we studied sp^3d and in VBT we studied sp^3.

Ex. IF_5

I containing = 7 $Ve^{\ominus}$

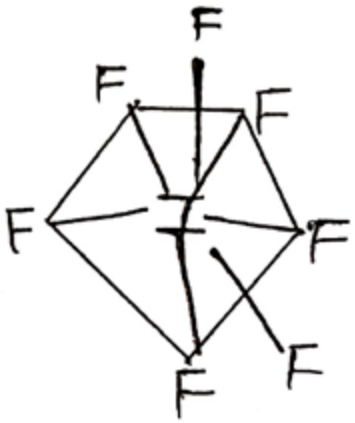
X – F
X – F
X – F
X – F
X – F
X
X] 1·P

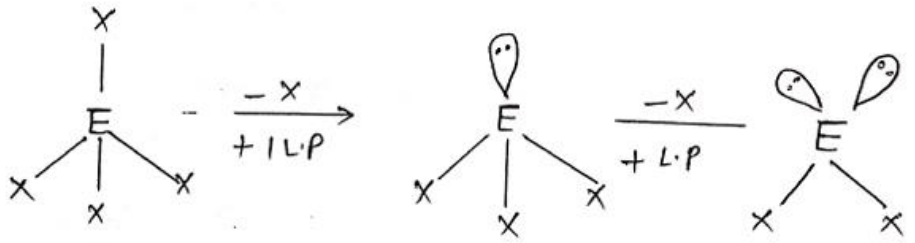
5 B·P + 1 L·P = 6 EP

Hybⁿ = sp^3d^2

Geometry = Octahedral

shape = Sq. pyramidal





4B·P + 0·LP = 4EP

Hybⁿ = sp^3

Geometry = Td

Shape = Td (B/c No L·P)

Identical Td

All bond angle and bond length are (same)

3B·P + 1L·P = 4EP

Hybⁿ = sp^3

Geometry = Td

Shape = Trigonal Pyramidal

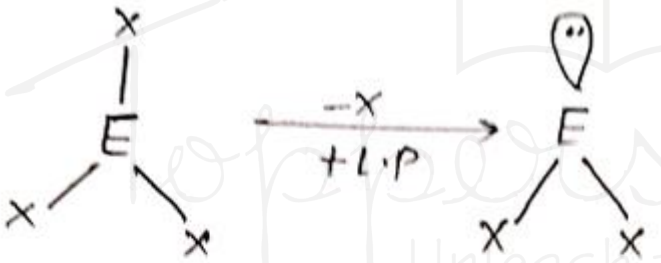
2B·P + 2L·P = 4EP

Hybⁿ = sp^3

Geometry = Td

Shape = Bent shape.

- ✓ If bond angle and all bond length are same we use identical word.



E·P = 3B·P + 0·L·P

EP = 3EP

Hybⁿ = sp^2

Geometry = Trigonal planer

Shape = Trigonal planer

2B·P + 1L·P = 3E·P

Hybⁿ = sp^2

Geometry = Trigonal planer

Shape = bent

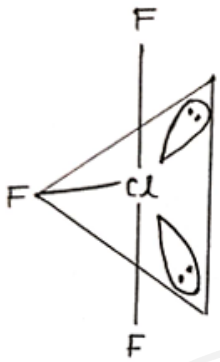
- **Bent Rule:-**
  - ✓ Bent rule applicable For T.B.P Geometry and sp^3d^3 hybridisation.
  - ✓ According to bent rule In T.B.P molecule more electronegative element present in axial position and less electronegative element present in equatorial position.
  - ✓ A/c to bent rule larger size element and molecules

Ex. ClF_3

$Cl = 7ve^{\ominus}$

X – F
X – F
X – F
X]1·P
X]1·P

3B·P + 2L·P
= 5EP
$Hyb^n = sp^3d$
Geo = T·B·P
Shape = T-shape

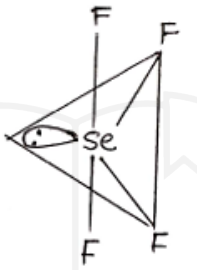


Ex · SeF_4

$Se = 6ve^{\ominus}$

X – F
X – F
X – F
X – F
X]1·P

4B·P + 1L·P
= 5EP
$Hyb^n = sp^3d$
Geo = T·B·P
Shape = See-saw

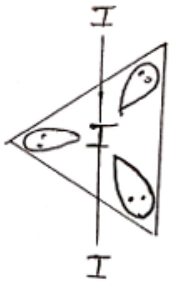


Ex. $I_3^{\ominus}$

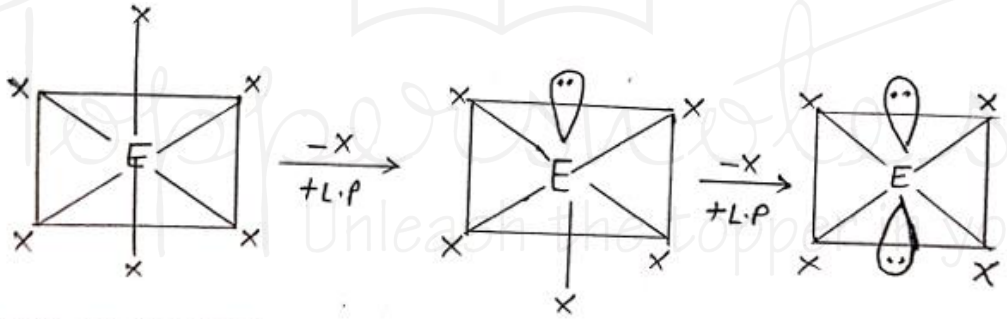
$I = 7ve^{\ominus} + 1(-ve)$

X – I
X – I
X]1·P
X]1·P
X]1·P

2B·P + 3L·P
= 5EP
$Hyb^n = sp^3d$
Geo = T·B·P
Shape = linear



Ex.

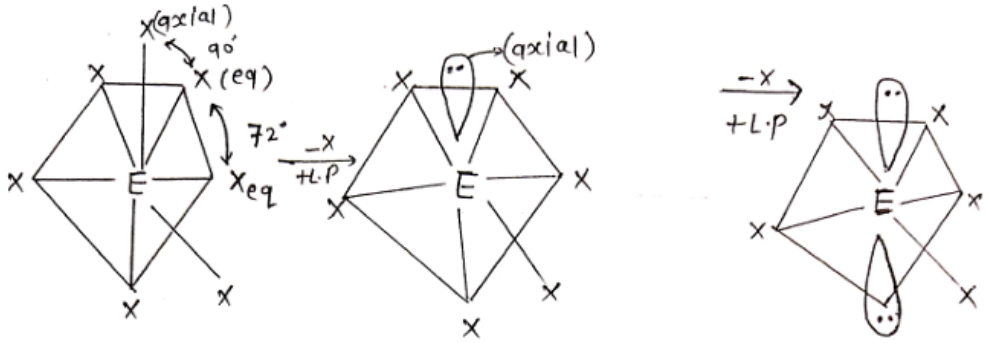


6B·P + 0·LP = 6EP
$Hyb^n = sp^3d^2$
Geo = oh
Shape = oh
Ex. SF_6 (Identical oh)

5B·P + 1L·P = 6EP
$Hyb^n = sp^3d^2$
Geo = oh
Shape = Sq. pyramidal
Ex. IF_5

4B·P + 2L·P = 6EP
$Hyb^n = sp^3d^2$
Geo = oh
Shape = Sq. planer
Ex. XeF_4, ICl

✓ IF Electron pair = 7 $Hyb^n = sp^3d^3$ Geometry = P.B.P



Que. Find out geometry shape, Hybridisation, bond pair and lone pair?

(i) XeO_4

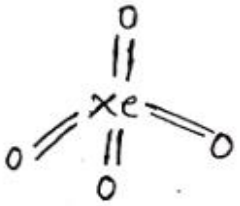
Xe = 8ve⊖

4BP + 0LP = 4EP

Hybⁿ = sp^3

Geo = Td

shape = Td



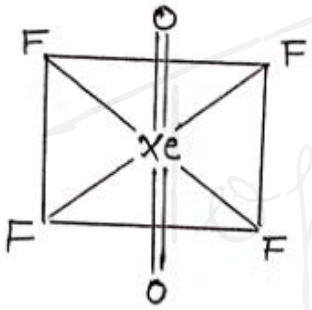
(ii) XeO_2F_4 Xe = 8 ve^-

6 B.P + 0 L.P = 6 EP

Hybⁿ = sp^3d^2

Geo = P.B.P

shape = oh (octahedral)



(iii)XeO_2F_2 Xe = 8 ve^-

Xe = 8ve⊖

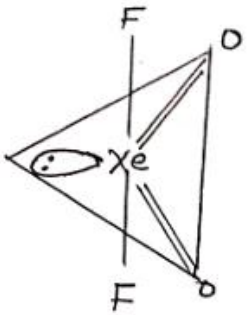
4 B.P + 1 L.P = 5EP

Hybⁿ = sp^3d

Geo = T.B.P

Use bent rule

shape = See-Saw



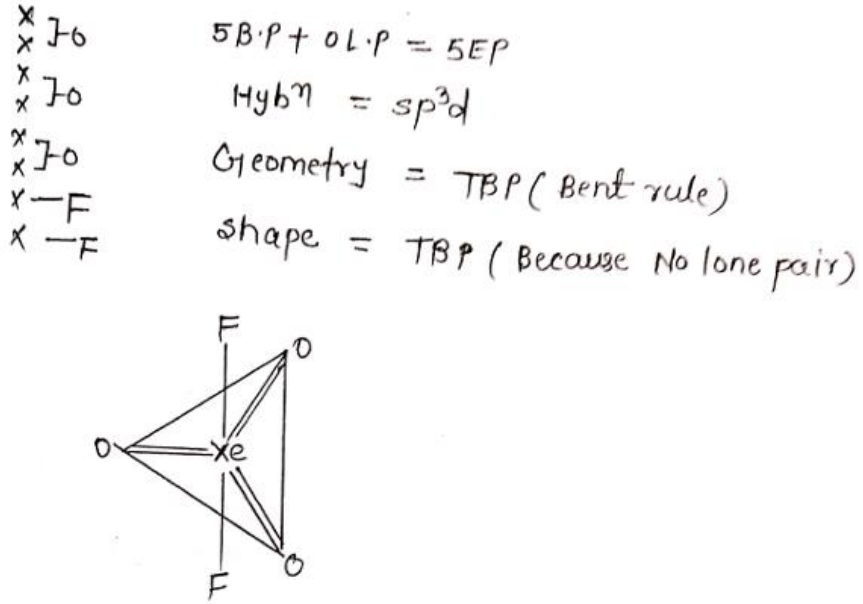
(iv)$[H_2F]^-$ 8 ve^-

2 B.P + 3 L.P = 5 E.P

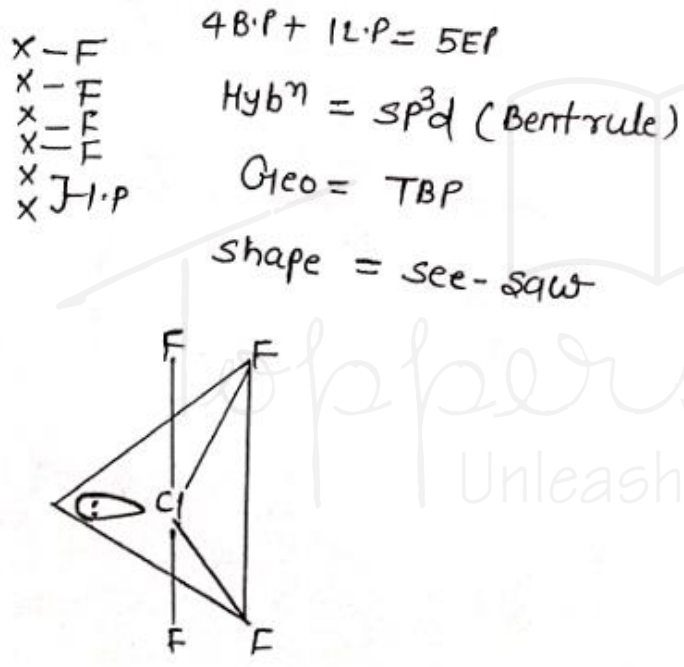
Geo = T.B.P

shape = linear shape

* **XeO_3F_2**



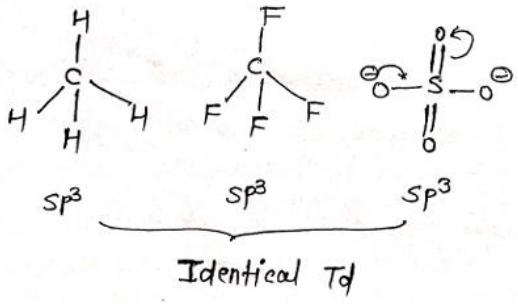
* **$[ClF_4]^+$**

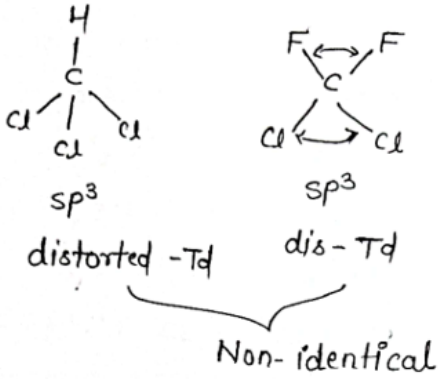


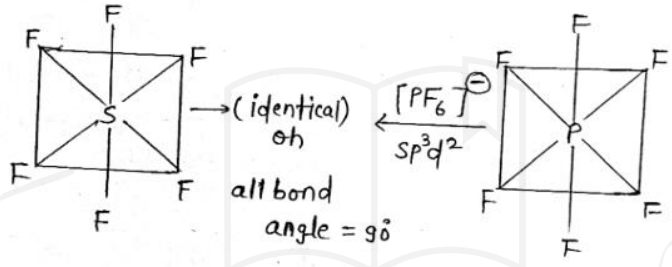
➢ **Shape:-**

1 L.P + 2 B.P = Bent shape
2 L.P + 2 B.P = Bent shape
1 L.P + 3 B.P = Pyramidal
1 L.P + 4 B.P = See-saw
2 L.P + 3 B.P = T-shape
3 L.P + 2 B.P = linear
1 L.P + 5 B.P = sq. pyramidal
2 L.P + 4 B.P = sq. planar
1 L.P + 6 B.P = pentagonal mono pyramidal

➢ **Identical Td and Identical octahedral:-** All bond angle and bond length are same called identical octahedral.







- **Iso-structure and Iso-electronic:-**
  - ✓ **Condition For Iso-structure**
    (i) Same Hybridisation
    (ii) Same No. of Lone pair and bond pair
  - ✓ **Condition For isoelectronic:-**
    (i) Same number of valence e^-.

Que. How many molecules are iso-structure and iso-electronic?

Ex. (a) $NH_4^{\oplus}$ (b) $BH_4^{\ominus}$ (c) CH_4 which are iso-structure?

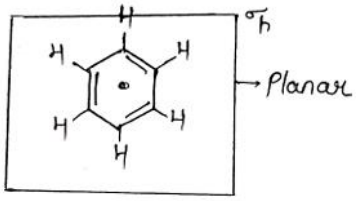
Ans.

$NH_4^{\oplus}$	$BH_4^{\ominus}$	CH_4
X – H	X – H	X – H
X – H	X – H	X – H
X – H	X – H	X – H
X – H	X – H	X – H
4 B.P = 4 EP	4 B.P = 4 EP	4 B.P + 0 L.P = 4 EP
Hyb^n = sp^3	Hyb^n = sp^3	Hyb^n = sp^3
Geo = Td	Geo = Td	Geometry = Td
shape = Td	Shape = Td	shape = Td
TVE = $8e^{\ominus}$	TVE = $8e^{\ominus}$	TVE = $8e^{\ominus}$

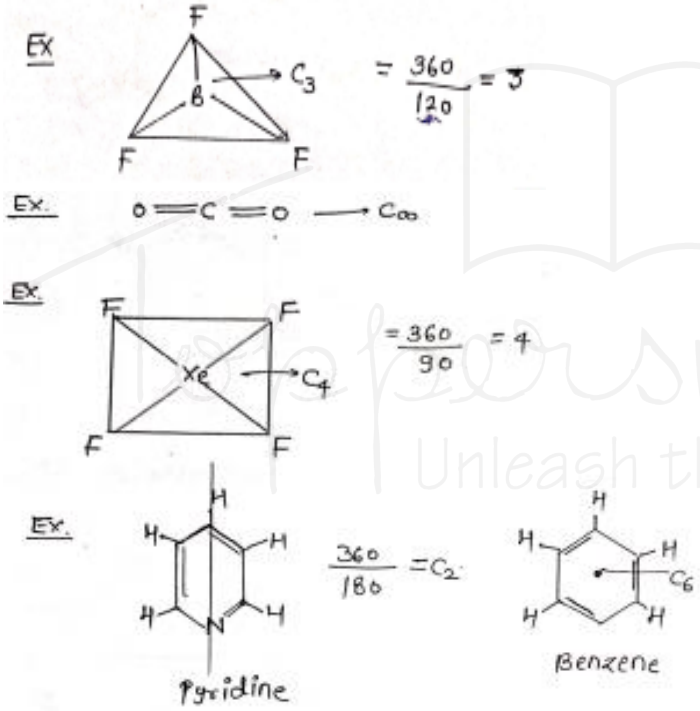
All are iso-str and isoelectronic

- **Planar or Non-Planar Molecule:**
  - ✓ Planar and non-planar nature of a molecule depends on symmetry.
  - ✓ If a molecule has a σ_h (horizontal) plane then it is planar.
  - ✓ If it has only σ_v (vertical plane) then it is non-planar.
  - ✓ Horizontal plane (σ_h) means a plane perpendicular to the principal axis.

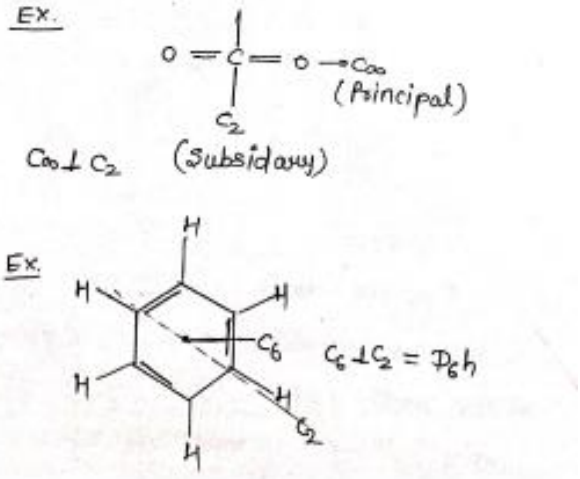
Ex. Benzene



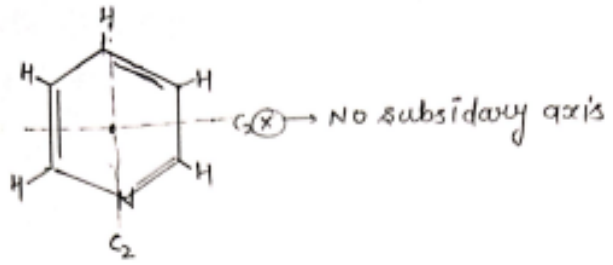
- **VSEPR VS Point group:** Point group depends on following factor.
  (i) principal axis (C_n)
  (ii) Subsidiary axis (C_2)
  (iii) Plane → $\sigma_h, \sigma_v, \sigma_d$
- **Principal axis (C_n):** Principal axis denote by C_n. n = Higher No. of rotation
  - ✓ The axis covered / shifted maximum atoms called **principal axis**.



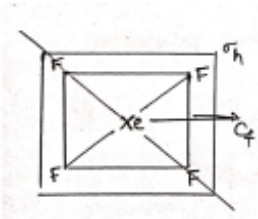
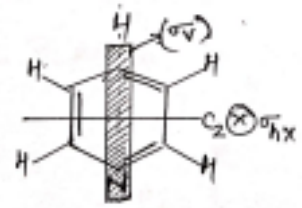
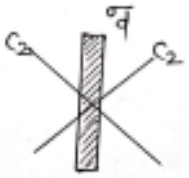
- **Subsidiary axis (C_2):** The axis perpendicular to principal axis.



Ex.

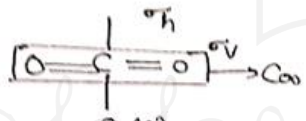


- **If principal axis (C_n) 1 subsidiary convert D_n.**

Plane		
σ_h	**σ_v**	**σ_d**
The plane 1 to C_n.	The plane $\parallel$ to Principal axis called vertical plane.	The plane bisect by two C_2-axis.
		
D_{4h} planar There is a subsidiary axis there will be a horizontal plane	**(Non-planar)** There is no subsidiary axis there will be a vertical plane.	These are generally found in organic molecules.

- ✓ If σ_h, σ_v and σ_d are all present in a molecule then the priority order will be as follows: $\sigma_h > \sigma_v > \sigma_d$.

Ex.



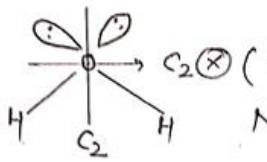
$C_n \perp C_2 = D_n$

$D_{\infty h}$ = planar

Whenever a subsidiary axis is perpendicular to the principal axis, it is converted into D_n.

If it is not perpendicular then C_n remains C_n.

Ex.

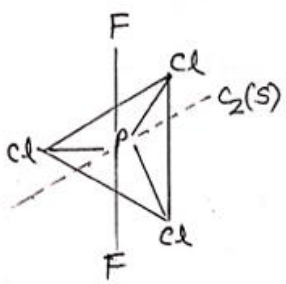


No horizental

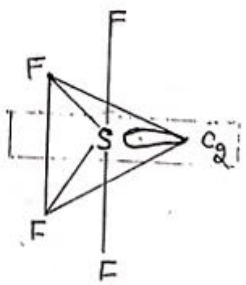
$C_2 \perp C_2(x) = C_{2v}$ (Non-planar)

- ✓ If a molecule has a σ_h plane, it is planar whereas molecules with σ_v planes are generally non-planar.

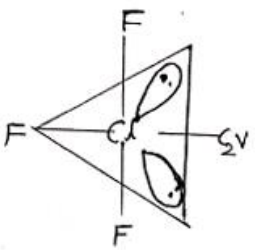
Ex.



$C_3 \perp C_2 = D_{3h}$ (Planar)



C_{2v} (Non-planar)

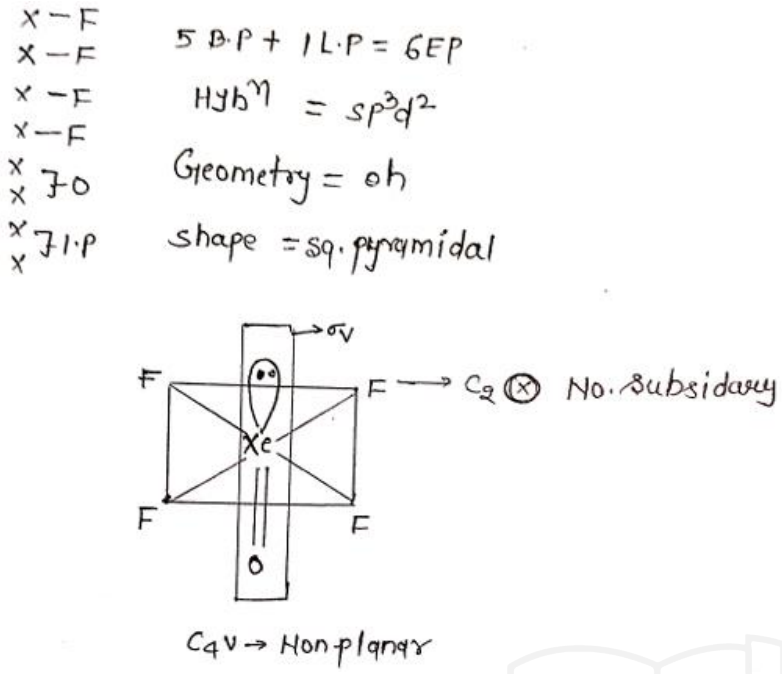


Sx hx (non-planar)

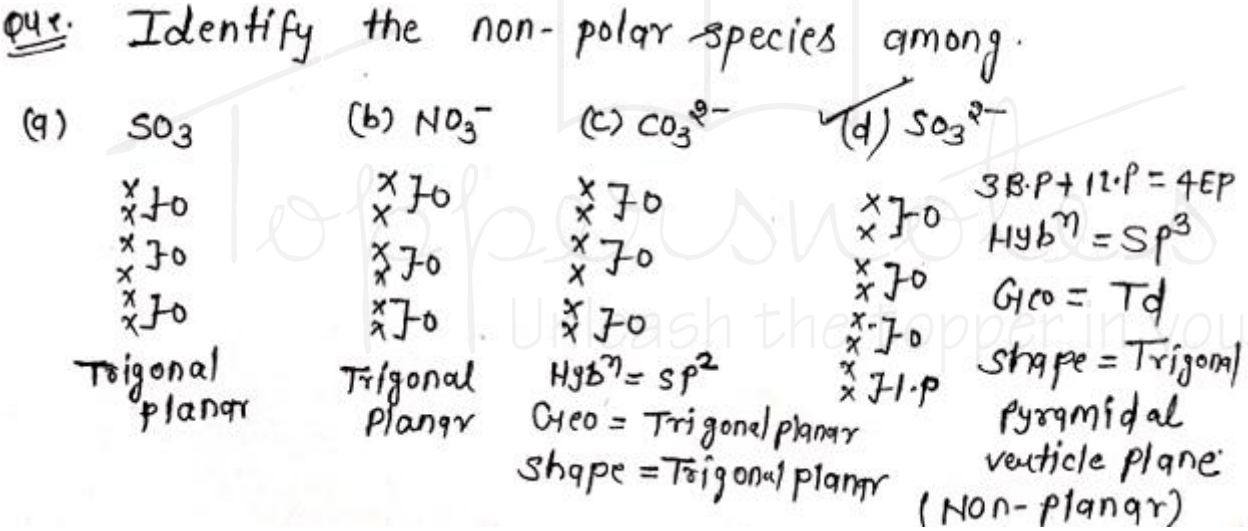
Que. The point group symmetry of $XeOF_4$ is

(a) D_{3h} (b) D_{4v} (c) C_{4v} (d) C_{3v}

Ans.



Whenever a pyramidal shape occurs there will always be a vertical plane.



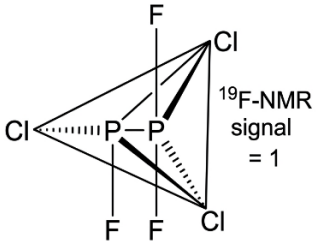
- **Tricks for point Group:**
  - ✓ Symmetrical linear: $D_{\infty h}$ point group (planar)
    Ex. CO_2 (sp)
  - ✓ Asymmetrical linear: $C_{\infty v}$ point group (Non-planar)
    Ex. (S=C=O) sp
  - ✓ Symmetrical Bent: C_{2v} (Non-planar)
    Ex. $OH_2, OF_2, O(CH_3)_2$
  - ✓ Symmetrical trigonal planar: D_{3h} (planar) → BF_3
  - ✓ Symmetrical pyramidal: C_{3v} (Non-planar)
    Ex. NH_3, NF_3, XeO_3
  - ✓ Symmetrical Td/oh: Tetrahedral (identical Td/oh) planar
    Ex. $CF_4, CH_4, XeO_4, SF_6, PF_6$
  - ✓ Symmetric TBP: D_{3h} (Planar)

➢ **VSEPR VS ^{19}FNMR, ^{31}PNMR, ^{11}BNMR signal and spectrum:**

Example:: PF_2Cl_3

X – Cl
X – Cl
X – Cl
X – F
X – F

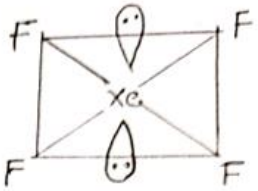
5 B.P = 5 EP
Hybn = sp^3d
Geo = T.B.P (bent rule)
Shape = T.B.P



Ex. XeF_4

X – F
X – F
X – F
X – F
X lp
X lp

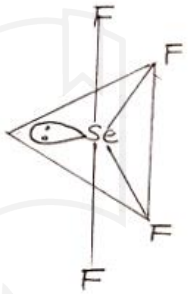
4 B.P + 2 L.P = 6 EP
Hybn = sp^3d^2
Geometry = oh
shape = sq. planar
^{19}F NMR signal = 1



Ex. SeF_4

X – F
X – F
X – F
X – F
X lp

4 B.P + 1 L.P = 5 EP
Hybn = sp^3d
Geo = TBP
shape = See-Saw
^{19}F NMR signal = 2

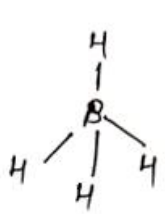


NMR (Nuclear Magnetic resonance)	
Active	**Inactive**
$^{A}_{Z}E \begin{pmatrix} A = \text{odd} \\ Z = \text{odd} \end{pmatrix} \begin{pmatrix} A = \text{even} \\ Z = \text{odd} \end{pmatrix} \begin{pmatrix} A = \text{odd} \\ Z = \text{even} \end{pmatrix}$	$^{A}_{Z}E \begin{pmatrix} A = \text{even} \\ Z = \text{even} \end{pmatrix}$
Nuclear spin $I \neq 0$	Nuclear spin I = 0
Ex. $^{1}H_1, ^{2}H_1, ^{19}F_9, ^{31}P_{15}, ^{11}B_5$	**Ex.** $^{12}_{6}C$, $^{24}_{12}Mg$

Ex. $[BH_4]^-$

X – H
X – H
X – H
X – H

4 EP
Hybn = sp^3
Geo = Td
shape = Td



^{1}HNMR signal = 1
^{11}BNMR signal = 1

^{11}BNMR spectrum = $2nI+1$
$= 2 \times 4 \times \frac{1}{2} + 1 = 5$ (quintet)

^{1}HNMR spectrum = $2nI+1$
$= 2 \times 1 \times \frac{3}{2} + 1 = 4$ (quartet)

Ex. $[PF_6]^{\ominus}$

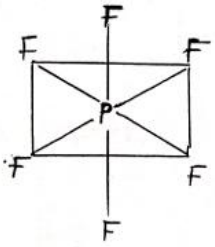
X – F
X – F
X – F
X – F
X – F
X – F

6 EP -

Hyb^n = sp^3d^2

Geo = octahedral

Shape = octahedral



^{19}F- NMR signal = 1

^{31}P NMR signal = 1

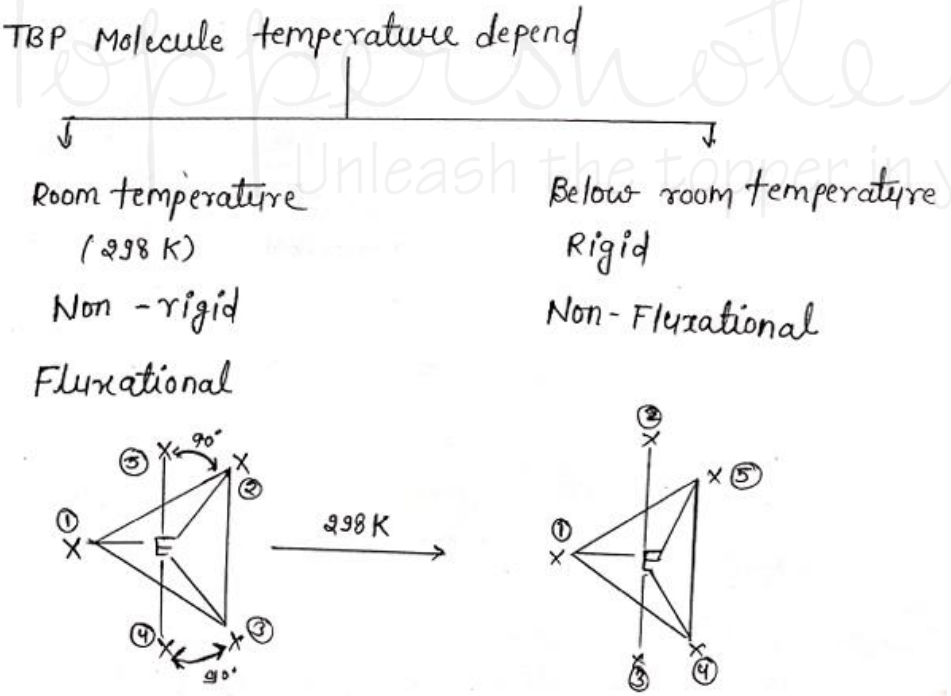
^{31}P- NMR spectrum = $2nI+1$

$= 2 \times 6 \times \frac{1}{2} + 1 = 7$ (septet)

^{19}F- NMR spectrum = $(2nI+1)$

$= 2 \times 1 \times \frac{1}{2} + 1 = 2$ (doublet)

- **Berry-pseudo rotation**
  - ✓ Berry pseudo rotation is applicable only for TBP (Trigonal Bipyramidal) molecules and sp^3d hybridization.
  - ✓ TBP molecules are temperature dependent, but identical geometries are temperature independent.
  - ✓ In identical TBP all positions are equivalent so only one signal is observed.
  - ✓ In Berry pseudo rotation axial bond inter convert into eq. bond and equatorial bond convert into axial bond at 90°.



  - ✓ Atom (2) and (3) are axial site and (4) and (5) is equatorial site.
  - ✓ Atom (4) and (5) are axial site and (2) and (3) are equatorial site.
  - ✓ Below room temperature berry-pseudo rotation not possible.
  - ✓ In between a transition state is formed which has a square-based pyramidal geometry.
  - ✓ Its point group is C_4v.
  - ✓ square base pyramidal —$sp^3dx^2\text{-}y^2$